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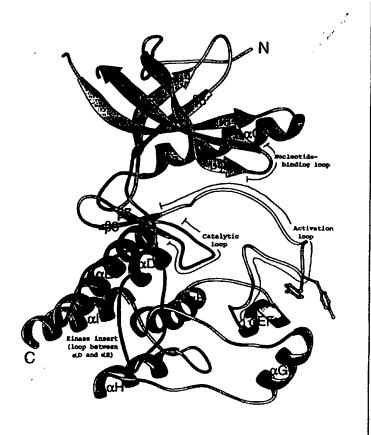
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(54) Title: CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

(57) Abstract

The present invention relates to the threedimensional structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates that define the structures of the protein tyrosine kinase and any of the compounds bound to it are pertinent to methods for determining the three-dimensional structures of protein tyrosine kinases with unknown structure and to methods that identify modulators of protein tyrosine kinase functions.



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DESCRIPTION

CRYSTAL STRUCTURES OF A PROTEIN TYROSINE KINASE

5 <u>RELATED APPLICATIONS</u>

This application is related to U.S. Application
Serial No. 08/701,191, by Mohammadi, et al., entitled
"Crystals of the Tyrosine Kinase Domain of Non-Insulin
Receptor Tyrosine Kinases," filed August 21, 1996 (Lyon
Lyon Docket No. 227/088) and U.S. Application Serial
No. 60/034,168, by McMahon, et al., entitled "Crystal
Structures of a Protein Tyrosine Kinase Complexed with
Compounds of the Oxindolinone/Thiolindolinone Family,"
filed December 19, 1996 (Lyon & Lyon Docket No.

221/282), which are hereby incorporated herein by
reference in their entirety including any drawings,
tables, and figures.

INTRODUCTION

The present invention relates to the three dimensional structures of protein kinases.

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BACKGROUND OF THE INVENTION

The following description of the background of the invention is provided simply as an aid in understanding the invention and is not admitted to describe or constitute prior art to the invention.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes (for a review, see Schlessinger and Ullrich, 1992, Neuron 9: 383-391). The PTK family contains multiple subfamilies, one of which

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is the fibroblast growth factor receptor (FGF-R) subfamily (for a review, see Givol and Yayon, 1992, FASEB J. 6 (15): 3362-3369).

All PTKs enzymatically transfer a high energy 5 phosphate from adenosine triphosphate to a tyrosine residue in a target protein. These phosphorylation events regulate cellular phenomena in signal transduction processes. Cellular signal transduction processes contain multiple steps that convert an 10 extracellular signal into an intracellular signal. intracellular signal is then converted into a cellular response. PTKs are components in many signal transduction processes. A PTK regulates the flow of a signal in a particular step in the process by 15 phosphorylating a downstream molecule. The addition of a phosphate can either modulate the activity of the downstream molecule by turning it "on" or "off". Thus, aberrations in a particular PTK's activity can either cause overflow or underflow of the signal. Overflow of 20 a signal can lead to such abnormalities as uncontrolled cell proliferation, which is representative of such disorders as cancer and angiogenesis.

Scientists in the biomedical community are searching for PTK inhibitors that down-regulate overflow signal transduction pathways. In particular, small molecule PTK inhibitors are sought that can traverse the cell membrane and not become hydrolyzed in acidic environments. These small molecule PTK inhibitors can be highly bioavailable and can be administered orally to patients.

Some small molecule PTK inhibitors have already

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been discovered. For example, bis(monocyclic), bicyclic or heterocyclic aryl compounds (PCT WO 92/20642), vinylene-azaindole derivatives (PCT WO 94/14808), 1-cyclopropyl-4-pyridyl-quinolones (U.S. Patent No. 5,330,992), styryl compounds (U.S. Patent No. 5,217,999), styryl-substituted pyridyl compounds (U.S. Patent No. 5,302,606), certain quinazoline derivatives (EP Application No. 0 566 266 Al), seleoindoles and selenides (PCT WO 94/03427), tricyclic polyhydroxylic compounds (PCT WO 92/21660), and benzylphosphonic acid compounds (PCT WO 91/15495) are described as PTK inhibitors.

Although many PTK inhibitors are known, many of these are not specific for PTK subfamilies and will therefore cause multiple side-effects as therapeutics. Compounds of the indolinone family, however, are specific for the FGFR subfamily and are non-hydrolyzable. WO 96/40116, "Indolinone Compounds for the Treatment of Disease," published December 19, 1996, inventors Tang et al. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, they are not complexed with PTK subfamily specific, hydrolysis resistant, small molecules.

Despite recent advances, the need remains in the art for crystallographic analysis of protein kinases, so that improved therapeutic molecules can be designed and synthesized.

30 <u>SUMMARY OF THE INVENTION</u>

The present invention relates to the three

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dimensional structures of protein tyrosine kinases. The use of X-ray crystallography can define the three dimensional structure of protein tyrosine kinase at atomic resolution.

The three dimensional structures described herein elucidate specific interactions between protein tyrosine kinases and compounds bound to them. The coordinates that define the three dimensional structures of protein tyrosine kinases are useful for determining three dimensional structures of PTKs with unknown structure. In addition, the coordinates are also useful for designing and identifying modulators of protein tyrosine kinase function. These modulators are potentially useful as therapeutics for diseases, including (but limited to) cell proliferative diseases, such as cancer, angiogenesis, atherosclerosis, and arthritis.

Thus in a first aspect, the invention features a crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

The term "crystalline form," in the context of the invention, is a crystal formed from an aqueous solution comprising a purified polypeptide corresponding to the catalytic domain of a PTK. A crystalline form of a protein tyrosine kinase is characterized as being capable of diffracting x-rays in a pattern defined by one of the crystal forms depicted in Blundel et al., 1976, Protein Crystallography, Academic Press. A crystalline form of a protein kinase is not characterized as being capable of diffracting x-rays in a pattern analogous to a crystalline form consisting of primarily salt or primarily a compound, for example.

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The term "protein tyrosine kinase," or PTK, refers to an enzyme that transfers the high energy phosphate of adenosine triphosphate to a tyrosine residue located on a protein target.

A protein tyrosine kinase catalytic domain of the invention can originate from receptor protein tyrosine kinases that bind fibroblast growth factor (FGF). These protein tyrosine kinases are known as "FGFR" herein, and can relate to one member of the FGFR family, such as FGFR1.

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The term "catalytic domain" refers to the region of a protein that can exist as a separate entity from the The catalytic domain of a protein tyrosine protein. kinase is characterized as having considerable amino acid identity to the catalytic domain of other protein tyrosine kinases. Considerable amino acid identity preferably refers to at least 30% identity, more preferably at least 35% identity, and most preferably at least 40% identity. These degrees of amino acid identity refer to the identity between different protein tyrosine kinase families. Amino acid identity for members of a given protein tyrosine kinase family range from 55% to 90%. The catalytic domain may be functional as a separate entity. The catalytic domain of a protein tyrosine kinase is also characterized as a polypeptide that is soluble in solution.

The term "identity" identity as used herein refers to a property of sequences that measures their similarity or relationship. Identity is measured by dividing the number of identical residues in the two sequences by the total number of residues and

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multiplying the product by 100. Thus, two copies of exactly the same sequence have 100% identity, but sequences that are less highly conserved and have deletions, additions, or replacements have a lower degree of identity. Those skilled in the art will recognize that several computer programs are available for determining sequence identity.

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The term "functional" refers to the ability of a catalytic domain to convert a substrate into a product

by phosphorylating the substrate. The term "functional" also relates to the ability of a catalytic domain to bind natural binding partners. The catalytic region may comprise an N-terminal tail, a catalytic core, and a C-terminal tail. The catalytic core is a polypeptide

that can be functional in terms of catalysis. N- and C-terminal tails are polypeptide regions that may not confer appreciable functionality in terms of catalysis, but may confer functionality in terms of modulator specificity.

A polypeptide can exist as a catalytic domain eventhough it is not functional. For example, a polypeptide corresponding to a catalytic domain may not be functional if it does not harbor phosphate moieties in key areas. Multiple examples of phosphorylation-state dependent function are well documented in the art. Therefore, a catalytic domain can also exist without being functional. A measure of a protein kinase catalytic domain is a polypeptide that is homologous to other protein kinase catalytic domains.

The term "polypeptide" refers to an amino acid chain representing a portion of, or the entire sequence

of, amino acids comprising a protein.

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A preferred embodiment of the invention includes a crystalline form of a PTK that is a receptor PTK.

Receptors are proteins that straddle the inside and outside of the cell membrane. Receptor PTKs comprise an extracellular region, a transmembrane region, and an intracellular region comprising a catalytic domain.

Another preferred embodiment of the invention is the crystalline form of a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

Yet another preferred embodiment of the invention is the crystalline form of a PTK that is a non-receptor PTK. Non-receptor PTKs are located inside the cell and do not harbor extracellular or membrane-spanning polypeptides attached to the polypeptide corresponding to the catalytic domain. Non-receptor PTKs may harbor fatty acids or lipids, which can impart a membrane associated character to a PTK. In preferred embodiments of the invention, crystalline forms of non-receptor PTKs are selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In still another preferred embodiment, the invention features a crystalline form of a PTK that comprises a heavy metal atom. These types of crystals can be referred to as derivative crystals.

The term "derivative crystal" refers to a crystal where the polypeptide is in association with one or more heavy-metal atoms.

The term "association" refers to a condition of proximity between a chemical entity or compound, or

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portions or fragments thereof, and tyrosine kinase domain protein, or portions or fragments thereof. The association may be non-covalent, i.e., where the juxtaposition is energetically favored by, e.g., hydrogen-bonding, van der Waals, electrostatic or hydrophobic interactions, or it may be covalent.

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The term "heavy metal atom" refers to an atom that is a transition element, a lanthanide metal, or an actinide metal. Lanthanide metals include elements with atomic numbers between 57 and 71, inclusive. Actinide metals include elements with atomic numbers between 89 and 103, inclusive.

In a preferred embodiment, the invention features a crystal of an FGF receptor tyrosine kinase domain protein. The FGF receptor tyrosine kinase domain protein can relate to FGFR1.

The term "FGFR1" refers to one member of multiple receptor PTKs that are homologous to one another and bind FGF. In this context, the term "homologous" refers to at least 70% amino acid identity between two members of the FGFR family.

The term "FGFR1" can also refer to a mutant of human FGFR1 which is characterized by the amino acid sequence of SEQ ID NO:2. As compared to human FGFR1, FGFR1 contains the following amino acid substitutions: Cys-488 - Ala, Cys-584 - Ser, Leu-457 - Val, and has an additional five amino acid residues at the N-terminus (Ser-Ala-Ala-Gly-Thr).

The term "human FGFR1" refers to the tyrosine

kinase domain of human fibroblast growth factor receptor

("FGFR1") having the amino acid sequence of SEQ ID

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NO:1. Generally, human FGFR1 comprises a 310 amino acid residue fragment (residues 456 to 765) of human FGFR1.

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The term "mutant" refers to a polypeptide which is obtained by replacing at least one amino acid residue in a native tyrosine kinase domain with a different amino acid residue. Mutation can be accomplished by adding and/or deleting amino acid residues within the native polypeptide or at the N- and/or C-terminus of a polypeptide corresponding to a native tyrosine kinase domain having substantially the same three-dimensional structure as the native tyrosine kinase domain from which it is derived. By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2 Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the Co atoms of the native tyrosine kinase are included in the superposition. A mutant may have, but need not have, PTK activity.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 1.

The term "atomic structural coordinates" as used herein refers to a data set that defines the three dimensional structure of a molecule or molecules. Structural coordinates can be slightly modified and still render nearly identical three dimensional structures. A measure of a unique set of structural coordinates is the root-mean-square deviation of the

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resulting structure. Structural coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed by a person of ordinary skill in the art as identical. Hence, the structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 are not limited to the values defined therein.

In other preferred embodiments, the invention features a crystalline form of the polypeptide in association with a compound. These types of crystalline forms can be referred to as co-crystals. The compound may be a cofactor, substrate, substrate analog, inhibitor, or allosteric effector.

The term "compound" refers to an organic molecule. The term "organic molecule" refers to a molecule which has at least one carbon atom in its structure. The compound can have a molecular weight of less than 6kDa. Both the geometry of the compound and the interactions formed between the compound and the polypeptide preferably govern high affinity binding between the two molecules. High affinity binding is preferably governed by a dissociation equilibrium constant on the order of 10⁻⁶ M or less. The compound is preferably a modulator that alters the function of a PTK.

The term "function," in reference to the effect of a modulator on PTK function, refers to the ability of a modulator to enhance or inhibit the catalytic activity of a PTK.

The term "catalytic activity", in the context of
the invention, defines the ability of a PTK to
phosphorylate a substrate polypeptide. Catalytic

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activity can be measured, for example, by determining the amount of a substrate converted to a product as a function of time. The conversion of the substrate to a product occurs at the active-site of the PTK.

The term "active-site" refers to a cavity located in the PTK in which one or more substrate molecules may bind. Addition of a modulator to cells expressing a PTK may enhance (activate) or lower (inhibit) the catalytic activity of the PTK.

A small number of inhibitors of PTK catalytic activity are known in the art. Small molecule inhibitors may modulate PTK function by blocking the binding of substrates. Indolinone compounds, for example, may bind to the active-site of PTK catalytic domains and inhibit them effectively, as measured by inhibition constants on the order of 10-6 M or less.

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Activators of PTK intracellular regions can enhance PTK function by interacting with both the PTK catalytic domain and the substrate. Activators may also promote dimerization of PTKs and thus activate them by bringing them into close proximity with one another. In addition, activators may operate by promoting a conformational change in the intracellular region of the PTK such that the catalytic region modifies substrates at a faster rate in the presence of the activator.

The term "function" can also refer to the ability of a modulator to enhance or inhibit the association between a PTK and a natural binding partner.

The term "natural binding partner" refers to a polypeptide that normally binds to a PTK in a cell.

These natural binding partners can play a role in

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propagating a signal in a PTK signal transduction process. The natural binding partner can bind to a PTK with high affinity. High affinity represents an equilibrium binding constant on the order of 10⁻⁶ M or less. However, a natural binding partner can also transiently interact with a PTK and chemically modify it. PTK natural binding partners are chosen from a group consisting of, but not limited to, src homology 2 (SH2) or 3 (SH3) domains, other phosphoryl tyrosine binding (PTB) domains, nucleotide exchange factors, and other protein kinases or protein phosphatases.

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The term "interactions" refers to hydrophobic, aromatic, and ionic forces and hydrogen bonds formed between atoms in the modulator and the enzyme activesite.

The term "cofactor" refers to a compound that may, in addition to the substrate, bind to a protein and undergo a chemical reaction. Multiple co-factors are nucleotides or nucleotide derivatives, such as phosphate and nicotinamide derivatives of adenosine.

The term "substrate" refers to a compound that reacts with an enzyme. Enzymes can catalyze a specific reaction on a specific substrate. For example, PTKs can phosphorylate specific protein and peptide substrates on tyrosine moieties. In addition, nucleotides can act as substrates for protein kinases.

The term "substrate analog" refers to a compound that is structurally similar, but not identical, to a substrate. The substrate analog may be a nucleotide analog. Examples of nucleotide analogs are described below.

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The term "inhibitor" refers to a compound that decreases the cellular function of a protein kinase. The protein kinase function is preferably the interaction with a natural binding partner and more preferably catalytic activity.

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The term "allosteric effector" refers to a compound that causes allosteric interactions in a protein. The term "allosteric interactions" refers to interactions between separate sites on a protein. The sites can be different from the active site. The allosteric effector can enhance or inhibit catalytic activity by binding to a site that may be different than the active site.

The term "co-crystal" refers to a crystal where the polypeptide is in association with one or more compounds.

In preferred embodiments, a co-crystal of the invention can be in association with a heavy metal atom. Examples of heavy metal atoms are described above.

In other preferred embodiments, the invention features a co-crystal comprising the crystalline form of the polypeptide in association with a compound, where the compound is a non-hydrolyzable analog of ATP. These analogs can be referred to as nucleotide analogs.

The term "ATP" refers to the chemical compound adenosine triphosphate.

The term "non-hydrolyzable" refers to a compound having a covalent bond that does not readily react with water. Examples of non-hydrolyzable analogs of ATP are AMP-PNP and AMP-PCP, whose structures are well known to those skilled in the art.

The term "AMP-PNP" refers to adenylyl

imidodiphosphate, a non-hydrolyzable analog of ATP.

The term "AMP-PCP" refers to adenylyl diphosphonate, a non-hydrolyzable analogue of ATP.

In another preferred embodiment, the invention relates to a crystalline form defined by the structural coordinates set forth in Table 2.

In preferred embodiments, the invention relates to crystalline forms, where the compound in association with the polypeptide is an indolinone.

10 Certain indolinones are specific modulators of PTK function. A preferred embodiment of the invention is the crystalline form of a PTK complexed with an indolinone of formula I or II:

$$\begin{array}{c|c} R_3 & R_4 \\ \hline R_2 & \hline \\ R_5 & R_6 \\ \hline \\ R_6 & R_7 & R_1 \\ \hline \end{array}$$

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$$\begin{array}{c|cccc}
R_{5} & A_{1} & CR_{3} \\
R_{5} & A_{2} & R_{2} \\
R_{6} & A_{3} & R_{1} & R_{2}
\end{array}$$

$$\begin{array}{c|ccccc}
R_{5} & R_{2} & R_{2} \\
R_{6} & R_{7} & R_{1} & (II)
\end{array}$$

or a pharmaceutically acceptable salt, isomer,

metabolite, ester, amide, or prodrug thereof, where:

- (a) A_1 , A_2 , A_3 , and A_4 are independently carbon or nitrogen;
 - (b) R₁ is hydrogen or alkyl;
 - (c) R_2 is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
 - (d) R₃ is hydrogen;

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- (e) R₄, R₅, R₆, and R₇ are optionally present, and are either (i) independently selected from the group consisting of alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO₂NRR', SO₃R, SR, NO₂, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH₂)_nCO₂R, and CONRR' or (ii) any two adjacent R₄, R₅, R₆, and R₇ taken together form a fused ring with the aryl portion of the indole-based portion of the indolinone;
- (f) R₂', R₃', R₄', R₅', and R₆' are each
 independently selected from the group consisting of
 hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl,
 alkaryloxy, halogen, trihalomethyl, S(O)R, SO₂NRR', SO₃R,
 SR, NO₂, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH₂),CO₂R,

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and CONRR';

- (g) n is 0, 1, 2, or 3;
- (h) R is hydrogen, alkyl or aryl;
- (i) R' is hydrogen, alkyl or aryl; and
- 5 (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-10 oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, 15 alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO_2NRR' , SO_3R , SR, NO_2 , NRR', OH, CN, C(O)R, OC(O)R, NHC(0)R, $(CH_2)_nCO_2R$ or CONRR'.

The term "pharmaceutically acceptable salt" refers to those salts which retain the biological activity and properties of the free bases. Pharmaceutically acceptable salts can be obtained by reaction with inorganic acids such as hydrochloric acid, hydrobromic acid, sulfuric acid, nitric acid, phosphoric acid, methanesulfonic acid, ethanesulfonic acid, p-toluenesulfonic acid, salicylic acid and the like.

The term "prodrug" refers to an agent that is converted into the parent drug in vivo. Prodrugs may be easier to administer than the parent drug in some situations. For example, the prodrug may be bioavailable by oral administration but the parent is not, or the prodrug may improve solubility to allow for

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intravenous administration.

"Alkyl" refers to a straight-chain, branched or cyclic saturated aliphatic hydrocarbon. Preferably, the alkyl group has 1 to 12 carbons. More preferably, it is a lower alkyl of from 1 to 7 carbons, more preferably 1 to 4 carbons. Typical alkyl groups include methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tertiary butyl, pentyl, hexyl and the like. The alkyl group may be optionally substituted with one or more substituents are selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO₂, halogen, N(CH₃)₂ amino, and SH.

"Alkenyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon group containing at least one carbon-carbon double bond. Preferably, the alkenyl group has 2 to 12 carbons. More preferably it is a lower alkenyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkenyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO₂, halogen, N(CH₃)₂ amino, and SH.

"Alkynyl" refers to a straight-chain, branched or cyclic unsaturated hydrocarbon containing at least one carbon-carbon triple bond. Preferably, the alkynyl group has 2 to 12 carbons. More preferably it is a lower alkynyl of from 2 to 7 carbons, more preferably 2 to 4 carbons. The alkynyl group may be optionally substituted with one or more substituents selected from the group consisting of hydroxyl, cyano, alkoxy, =0, =S, NO₂, halogen, N(CH₃)₂ amino, and SH.

"Alkoxy" refers to an "O-alkyl" group.

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"Aryl" refers to an aromatic group which has at least one ring having a conjugated pi-electron system and includes carbocyclic aryl, heterocyclic aryl and biaryl groups. The aryl group may be optionally substituted with one or more substituents selected from the group consisting of halogen, trihalomethyl, hydroxyl, SH, OH, NO₂, amine, thioether, cyano, alkoxy, alkyl, and amino.

"Alkaryl" refers to an alkyl that is covalently joined to an aryl group. Preferably, the alkyl is a lower alkyl.

"Carbocyclic aryl" refers to an aryl group wherein the ring atoms are carbon.

"Heterocyclic aryl" refers to an aryl group having

from 1 to 3 heteroatoms as ring atoms, the remainder of
the ring atoms being carbon. Heteroatoms include
oxygen, sulfur, and nitrogen. Thus, heterocyclic aryl
groups include furanyl, thienyl, pyridyl, pyrrolyl, Nlower alkyl pyrrolo, pyrimidyl, pyrazinyl, imidazolyl
and the like.

"Amide" refers to -C(0)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

"Thioamide" refers to -C(S)-NH-R, where R is alkyl, aryl, alkylaryl or hydrogen.

25 "Amine" refers to a -N(R')R'' group, where R' and R'' are independently selected from the group consisting of alkyl, aryl, and alkylaryl.

"Thioether" refers to -S-R, where R is alkyl, aryl, or alkylaryl.

"Sulfonyl" refers to -S(O)₂-R, where R is aryl, C(CN)=C-aryl, CH₂CN, alkyaryl, sulfonamide, NH-alkyl, NH-

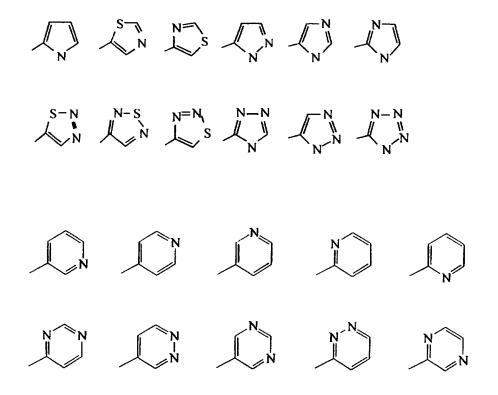
alkylaryl, or NH-aryl.

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The term "acyl" denotes groups -C(O)R, where R is alkyl as defined above, such as formyl, acetyl, propionyl, or butyryl.

It is understood by those skilled in the art that when A_1 , A_2 , A_3 , and A_4 are nitrogen or sulfur that the corresponding R_4 , R_5 , R_6 , and R_7 , as well as the corresponding bond, do not exist.

Examples of indoles having such fused rings (as described in (e) (ii) above include the following:



The six membered rings shown above exemplify possible A rings in compound II.

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Other preferred embodiments of the invention are crystalline forms comprising 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone as well as 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone. The polypeptide of these crystalline forms can be FGFR, and specifically, FGFR1.

In preferred embodiments, the crystalline forms of the invention can be defined by the structural coordinates set forth in Table 3 or Table 4.

The use of X-ray crystallography can elucidate the three dimensional structure of crystalline forms of the invention. The first characterization of crystalline forms by X-ray crystallography can determine the unit cell shape and its orientation in the crystal.

In other preferred embodiments, the invention features a crystal of an FGF receptor tyrosine kinase domain protein, where the crystal is characterized by having monoclinic unit cells. The crystal may also be characterized by having space group symmetry C2.

The term "unit cell" refers to the smallest and simplest volume element (i.e., parallelpiped-shaped block) of a crystal that is completely representative of the unit of pattern of the crystal. The dimensions of the unit cell are defined by six numbers: dimensions a, b and c and angles α , β and γ . A crystal can be viewed as an efficiently packed array of multiple unit cells. Detailed descriptions of crystallographic terms are described in, which is hereby incorporated herein by reference in its entirety, including any drawings, figures, and tables.

The term "monoclinic unit cell" refers to a unit

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cell where a \neq b \neq c; α = γ = 90°; and β > 90°.

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The term "space group" refers to the symmetry of a unit cell. In a space group designation (e.g., C2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance.

The term "lattice" in reference to crystal structures refers to the array of points defined by the vertices of packed unit cells.

The term "symmetry operations" refers to geometrically defined ways of exchanging equivalent parts of a unit cell, or exchanging equivalent molecules between two different unit cells. Examples of symmetry operations are screw axes, centers of inversion, and mirror planes.

In a preferred embodiment, the invention features a crystalline form, where the monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and $B=107.2^{\circ}$.

In a preferred embodiment, the invention features a FGFR1 crystal, where the monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and β =107.7°.

In another aspect the invention features a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase, containing at least about 20 amino acid residues upstream of the first glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal

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boundary of the catalytic domain.

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The polypeptides of the invention can be isolated, enriched or purified. In addition, the crystalline forms of the invention can be formed from polypeptides that are isolated, enriched, or purified.

By "isolated" in reference to a polypeptide is meant a polymer of 6, 12, 18 or more amino acids conjugated to each other, including polypeptides that are isolated from a natural source or that are synthesized. The isolated polypeptides of the present invention are unique in the sense that they are not found in a pure or separated state in nature. Use of the term "isolated" indicates that a naturally occurring sequence has been removed from its normal cellular environment. Thus, the sequence may be in a cell-free solution or placed in a different cellular environment. The term does not imply that the sequence is the only amino acid chain present, but that it is essentially free (about 90 - 95% pure at least) of material naturally associated with it.

By the use of the term "enriched" in reference to a polypeptide it is meant that the specific amino acid sequence constitutes a significantly higher fraction (2 - 5 fold) of the total of amino acids present in the cells or solution of interest than in normal or diseased cells or in the cells from which the sequence was taken. This could be caused by a person by preferential reduction in the amount of other amino acids present, or by a preferential increase in the amount of the specific amino acid sequence of interest, or by a combination of the two. However, it should be noted that "enriched"

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does not imply that there are no other amino acid sequences present, just that the relative amount of the sequence of interest has been significantly increased. The term significant here is used to indicate that the level of increase is useful to the person making such an increase, and generally means an increase relative to other amino acids of about at least 2 fold, more preferably at least 5 to 10 fold or even more. The term also does not imply that there are no amino acids from other sources. The other source amino acids may, for example, comprise amino acids encoded by a yeast or bacterial genome, or a cloning vector such as pUC19. The term is meant to cover only those situations in which a person has intervened to elevate the proportion of the desired nucleic acid.

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It is also advantageous for some purposes that an amino acid sequence be in purified form. The term "purified" in reference to a polypeptide does not require absolute purity (such as a homogeneous preparation); instead, it represents an indication that the sequence is relatively purer than in the natural environment (compared to the natural level this level should be at least 2-5 fold greater, e.g., in terms of mg/ml). Purification of at least one order of magnitude, preferably two or three orders, and more preferably four or five orders of magnitude is expressly contemplated. The substance is preferably free of contamination at a functionally significant level, for example 90%, 95%, or 99% pure.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a

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receptor PTK. The receptor PTK may have a threedimensional structure substantially similar to that of the insulin receptor, even though the amino acid content may be different.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, where the non-insulin receptor tyrosine kinase is a cytoplasmic tyrosine kinase.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a receptor PTK, selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, or MUSK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a non-receptor PTK, selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, or ACK.

In a preferred embodiment, the invention features a polypeptide corresponding to the catalytic domain of a PTK, having the amino acid sequence shown in Table 1 or Table 2.

In another aspect, the invention features a method for creating crystalline forms described herein. The method may utilize the polypeptides described herein to form a crystal. The method comprises the steps of:

- (a) mixing a volume of polypeptide solution with a reservoir solution; and
- (b) incubating the mixture obtained in step(a) over the reservoir solution in a closed container,under conditions suitable for crystallization.

These processes are described in detail in the

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section entitled "Detailed Description of the Invention."

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In another aspect, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of: (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, where the polypeptide solution comprises 1 mg/mL to 60 mg/mL FGFtype tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and where the reservoir solution comprises 10% to 30% (w/v) polyethylene glycol. 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and (b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25°C until crystals form.

In a preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

In another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine

kinase domain polypeptide in crystalline form, where the polypeptide solution includes a compound such as a cofactor, substrate, substrate analog, inhibitor or allosteric effector.

In still another preferred embodiment, the invention features a method of obtaining FGF receptor tyrosine kinase domain polypeptide in crystalline form, where the compound is a nucleotide analog, such as a non-hydrolyzable analog of ATP, or an indolinone.

Indolinone compounds have the general structural formula

Indolinone compounds have the general structural formula as described herein.

In another aspect, the invention features a cDNA encoding an FGF receptor tyrosine kinase domain protein, where a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.

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Another aspect of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure by utilizing the structural coordinates of Table 1, Table 2, Table 3, and Table 4. These methods can relate to homology modeling, molecular replacement, and nuclear magnetic resonance methods.

In a preferred embodiment, the invention relates to a method of determining three dimensional structures of PTKs with unknown structures by utilizing the coordinates of Table 1, Table 2, Table 3, or Table 4 in conjunction with the amino acid sequences of PTKs. This method of homology modeling comprises the steps of: (a) aligning the computer representation of an amino acid sequence of a PTK with unknown structure with that of a PTK with known structure, where alignment is achieved by matching homologous regions of the amino acid sequences;

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(b) transferring the computer representation of an amino acid structure in the PTK sequence of known structure to a computer representation of a structure of the corresponding amino acid in the PTK sequence with unknown structure; and (c) determining low energy conformations of the resulting PTK structure.

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The term "amino acid sequence" describes the order of amino acids in the amino acid chain comprising a polypeptide corresponding to the catalytic domain of a PTK.

The term "aligning" describes matching the beginning and the end of two or more amino acid sequences. Homologous amino acid sequences are placed on top of one another during the alignment process.

The term "homologous" describes amino acids in two sequences that are identical or have similar side-chain chemical groups (e.g., aliphatic, aromatic, polar, negatively charged, or positively charged).

The term "corresponding" refers to an amino acid that is aligned with another in the sequence alignment mentioned above.

The term "determining the low energy conformation" describes a process of changing the conformation of the PTK structure such that the structure is of low free energy. The PTK structure may or may not have molecules, such as modulators bound to it.

The term "low free energy" describes a state where the molecules are in a stable state as measured by the process. A stable state is achieved when favorable interactions are formed within the complex.

The term "favorable interactions" refers to

hydrophobic, aromatic, and ionic forces, and hydrogen bonds.

Another preferred embodiment of the invention relates to a method of determining three dimensional structures of PTKs with unknown structure. This method is accomplished by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to an incomplete X-ray crystallographic data set for a PTK. The method comprises the steps of: (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals, where one data set is complete and the other is incomplete; and (b) determining a low energy conformation of the resulting PTK structure.

The term "incomplete data set" relates to a X-ray crystallographic data set that does not have enough information to give rise to a three dimensional structure.

relates to a method of determining three dimensional structures of PTKs with unknown structure by applying the structural coordinates of Table 1, Table 2, Table 3, or Table 4 to nuclear magnetic resonance (NMR) data of a PTK. This method comprises the steps of: (a)

determining the secondary structure of a PTK structure using NMR data; and (b) simplifying the assignment of through-space interactions of amino acids. The PTK structure may not be complexed with compounds or modulators.

The term "secondary structure" describes the arrangement of amino acids in a three dimensional

structure, such as in α -helix or β -sheet elements.

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The term "through-space interactions" defines the orientation of the secondary structural elements in the three dimensional structure and the distances between amino acids from different portions of the amino acid sequence.

The term "assignment" defines a method of analyzing NMR data and identifying which amino acids give rise to signals in the NMR spectrum.

In another aspect, the invention features a method of identifying potential modulators of PTK function.

These modulators are identified by docking a computer representation of a structure of a compound with a computer representation of a cavity formed by the active-site of a PTK. The computer representation of the PTK active-site structure can be defined by structural coordinates.

The term "chemical group" refers to moieties that can form hydrogen bonds, hydrophobic, aromatic, or ionic interactions.

The term "docking" refers to a process of placing a compound in close proximity with a PTK. The term can also refer to a process of finding low energy conformations of the compound/PTK complex.

A preferred embodiment of the invention is a method of identifying potential modulators of PTK function.

The method involves utilizing the structural coordinates or a PTK three dimensional structure. The structural coordinates set forth in Table 1, Table 2, Table 3, and Table 4 can be utilized. The method comprises the steps of: (a) removing a computer representation of a PTK

structure and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the PTK; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying compounds that best fit the PTK active-site as potential modulators of PTK function. The initial PTK structure may or may not have compounds bound to it.

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The term "favorable geometric fit" refers to a conformation of the compound-PTK complex where the surface area of the compound is in close proximity with the surface area of the active-site without forming unfavorable interactions. Unfavorable interactions can be steric hindrances between atoms in the compound and atoms in the PTK active-site.

The term "favorable complementary interactions" relates to hydrophobic, aromatic, ionic, and hydrogen bond donating, and hydrogen bond accepting forces formed between the compound and the PTK active-site.

The term "potential" qualifies the term "modulator of PTK function" because the potential modulator or PTK function has not yet been tested for activity in vitro or in vivo.

The term "best fit" describes compounds that complexed the most surface area in the complex and/or form the most favorable complementary interactions with the PTK in the screen in a given experiment.

Another preferred embodiment of the invention is a method of identifying potential modulators of PTK function. The method involves utilizing a three

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dimensional structure of a PTK, with or without compounds bound to it. The method comprises the steps of: (a) modifying a computer representation of a PTK having one or more compounds bound to it, where the computer representations of the compound or compounds and PTK are defined by structural coordinates; (b) determining a conformation of the complex with a favorable geometric fit and favorable complementary interactions; and (c) identifying the compounds that best fit the PTK active-site as potential modulators of PTK function.

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The term "modifying" relates to deleting a chemical group or groups or adding a chemical group or groups.

Computer representations of the chemical groups can be selected from a computer data base.

Yet another preferred embodiment of the invention is a method of identifying potential modulators of PTK function by operating modulator construction or modulator searching computer programs on the compounds complexed with the PTK. The method comprises the steps of: (a) removing a computer representation of one or more compounds complexed with a PTK; and (b) searching a data base for compounds similar to the removed compounds using a compound searching computer program, or replacing portions of the compounds complexed with the PTK with similar chemical structures from a data base using a compound construction computer program, where the representations of the compounds are defined by structural coordinates.

The term "operating" as used herein refers to utilizing the three-dimensional conformation of

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molecules defined by the processes described herein in various computer programs.

The term "similar compound" refers to a compound in a computer data base that has a similar geometric structure as compounds that can bind to a PTK. The similar compound can also have similar chemical groups as the compounds that are either bound to the PTK or once bound to the PTK. The similar chemical groups can form complementary interactions with the PTK.

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The term "compound searching computer program"

describes a computer program that searches computer
representations of compounds from a computer data base
that have similar three dimensional structures and
similar chemical groups as a compound of interest. The
compound of interest is preferably an indolinone
compound.

The term "similar chemical structures" refers to chemical groups that share similar geometry as portions of the compounds in complex with the PTK or compounds removed from the PTK structure. Similar chemical structures can also refer to chemical groups that may form similar complementary interactions as portions of the compounds in complex with the PTK or compounds removed from the PTK structure.

The term "replacing structures" refers to removing a portion of the compounds in complex with the PTK or compounds removed from the PTK structure and connecting the broken bonds to a similar chemical structure.

The term "compound construction computer program" describes a computer program that replaces computer representations of chemical groups in a compound with

groups from a computer data base. The compound is preferably an indolinone compound.

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The term "similar three dimensional structure" describes two molecules with nearly identical shape and volume.

In another preferred embodiment of the invention, the PTK structures used in the modulator design or identification method of the invention are defined by the structural coordinates of Table 1, Table 2, Table 3, or Table 4.

The methods for using the crystalline forms and three dimensional structures of the invention can relate to a broad range of protein kinases. Thus, in preferred embodiments, the invention relates to a receptor PTK.

The receptor PTK can be selected form the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. The PTK may also exist as a non-receptor PTK. The non-receptor PTK can be selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

In another aspect, the invention features a potential modulator of PTK function identified by methods disclosed in the invention.

A preferred embodiment of the invention is that the potential modulator of PTK function is an oxindolinone or a thiolindolinone of formula I or II disclosed above.

Another aspect of the invention is a method for synthesizing a potential modulator of PTK function or its pharmaceutically acceptable salts, isomers, metabolites, esters, amides, or prodrugs by a standard

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synthetic method known in the art. Synthetic procedures are discussed below.

In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of PTK phosphorylation between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in the level of PTK phosphorylation.

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The term "cells" refers to any type of cells either primary or cultured. Primary cells can be extracted directly from an organism while cultured cells rapidly divide and can be cultured in many successive rounds. Cells can be grown in a variety of containers including, but not limited to flasks, dishes, and well plates.

The term "administer" refers to a method of delivering a compound to cells. The compound can be prepared using a carrier such as dimethyl sulfoxide (DMSO) in an aqueous solution. The aqueous solution comprising the compound, also termed an "aqueous preparation", can be simply mixed into the medium bathing the layer of cells or microinjected into the cells themselves. The compounds may be administered to the cells using a suitable buffered solution.

The term "suitable buffered solution" refers to an aqueous preparation of the compound that comprises a salt that can control the pH of the solution at low concentrations. Because the salt exists at low

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concentrations, the salt preferably does not alter the function of the cells.

The term "PTK phosphorylation" refers to the presence of phosphate on the PTK. Phosphates on PTKs can be identified by antibodies that bind them specifically with high affinity.

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In another aspect, the invention features a method of identifying a potential modulator of PTK function as a modulator of PTK function. The method comprises the steps of: (a) administering a potential modulator of PTK function to cells; (b) comparing the level of cell growth between cells not administered the potential modulator and cells administered the potential modulator; and (c) identifying the potential modulator as a modulator of PTK function based on the difference in cell growth.

The term "cell growth" refers to the rate at which a group of cells divides. Cell division rates can be readily measured by methods utilized by those skilled in the art.

Another aspect of the invention features a method of diagnosing a disease by identifying cells harboring a PTK with inappropriate activity. The method comprises the steps of: (a) administering a modulator of PTK function to cells; (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and (c) diagnosing a disease by characterizing cells harboring a PTK with inappropriate activity from the effect of the modulator on the difference in the rate of cell growth. The modulator can be identified by the methods of the

invention.

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The term "inappropriate activity" refers to a PTK that regulates a step in a signal transduction process at a higher or lower rate than normal cells.

Aberrations in the rate of signal transduction can be caused by alterations in the stimulation of a receptor PTK by a growth factor, alterations in the activity of PTK-specific phosphatase, over-expression of a PTK in a cell, or mutations in the catalytic region of the PTK itself.

The term "signal transduction process" describes the steps in a cascade of events where an extracellular signal is transmitted into an intracellular signal.

The term "PTK-specific phosphatase" describes an enzyme that dephosphorylates a particular PTK and thereby regulates that PTK's activity.

Another aspect of the invention is a method of treating a disease associated with a PTK with inappropriate activity in a cellular organism, where the method comprises the steps of: (a) administering the modulator of PTK function to the organism, where the modulator is in an acceptable pharmaceutical preparation; and (b) activating or inhibiting the PTK function to treat the disease.

The term "organism" relates to any living being comprised of at least one cell. An organism can be as simple as one eukaryotic cell or as complex as a mammal.

The term "administering", in reference to an organism, refers to a method of introducing the compound to the organism. The compound can be administered when the cells or tissues of the organism exist within the

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organism or outside of the organism. Cells existing outside the organism can be maintained or grown in cell culture dishes. For cells harbored within the organism, many techniques exist in the art to administer compounds, including (but not limited to) oral, parenteral, dermal, and injection applications. For cells outside of the patient, multiple techniques exist in the art to administer the compounds, including (but not limited to) cell microinjection techniques,

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The term "pharmaceutically acceptable composition" refers to a preparation comprising the modulator of PTK activity. The composition is acceptable if it does not appreciably cause irritations to the organism administered the compound.

Preferred embodiments of the of the invention are that the PTK is a receptor PTK selected from the group consisting of FGF-R, PDGF-R, FLK-1, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Other preferred embodiments of the invention are that the PTK is a non-receptor PTK selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

The summary of the invention described above is non-limiting and other features and advantages of the invention will be apparent from the following detailed description, and from the claims.

BRIEF DESCRIPTION OF THE FIGURES

FIG. 1 provides a ribbon diagram of the structure of FGFR1 showing the side chains of tyrosines Tyr-653

and Tyr-654 and the α helical (α C, α D, α E, α EF, α F- α I), β strand (β 1- β 5, β 7, β 8), nucleotide-binding loop, catalytic loop, activation loop and kinase insert regions of the molecule. The termini are denoted by N and C. The loop between β 2 and β 3 is disordered, indicated by a break in the chain in this region.

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FIG. 2 provides a stereo view of a C_o trace of FGFR1 shown in the same orientation as FIG. 1, with every tenth amino acid residue marked with a filled circle and every twentieth amino acid residue labeled with a residue number.

FIG. 3 provides a structure-based sequence alignment of human fibroblast growth factor receptor 1 (FGFR1), human fibroblast growth factor receptor 2 (FGFR2), human fibroblast growth factor receptor 3 (FGFR3), human fibroblast growth factor receptor 4 (FGFR4), a D. malanogaster homolog (DFGFR1), a C. elegans homolog (EGL-15) and insulin receptor tyrosine kinase (IRK).

FIGS. 4A and 4B provide ribbon diagrams of the N-terminal lobes (4A) and C-terminal lobes (4B) of FGFR1 and IRK in which the C_{α} atoms of the β sheets (4A) or α -helices (4B) of the two proteins have been superimposed.

FIG. 5 illustrates the side-chain positions of the tyrosine autophosphorylation sites of FGFR1 on the backbone representation of FGFR1.

FIGS. 6A and 6B are amino acid sequence alignments of the catalytic domains of PTKs, including receptor and non-receptor type PTKs. FIG. 6A depicts one representative member from each of the eighteen subfamilies of receptor tyrosine kinases. FIG. 6B

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depicts one representative member from each of the subfamilies of cytoplasmic tyrosine kinases. In FIGS. 6A and 6B highly conserved residues are boxed. The position of the glycine-rich domain, kinase insert, catalytic loop, and activation loop are indicated. The numbering is for human FGF-receptor.

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BRIEF DESCRIPTION OF THE CRYSTALLOGRAPHIC ATOMIC STRUCTURAL COORDINATES

10 The crystallographic structural coordinates are located at the end of the section entitled "Examples" and before the claims. Three sets of coordinates can be found in the Protein Data Bank under accession names 1FGK, 1AGW, and 1FGI. The 1FGK coordinates correspond to those listed in Table 1, the 1AGW coordinates correspond to those listed in Table 4, and the 1FGI coordinates correspond to those listed in Table 3. The 1AGW and 1FGI coordinate sets will be publically available in March 1998.

Table 1 provides the atomic structure coordinates of native FGFR1 crystals of the invention as determined by X-ray crystallography; and

Table 2 provides the atomic structure coordinates of FGFR1:AMP-PCP co-crystals of the invention as determined by X-ray crystallography.

Table 3 lists crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The columns (from left to right) are descriptions of the atoms by number and type, amino acid and number containing the atom, the x coordinate, y

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coordinate, z coordinate, bond connectivity, and temperature factor. All of these parameters are well defined in the art.

Table 4 is a file of crystallographic coordinates defining the three dimensional structure of FGF-R1 complexed with 3-[4-(4-formylpiperazine-1-yl) benzylidenyl]-2-indolinone. The columns are as described in Table 3.

10 <u>DETAILED DESCRIPTION OF THE INVENTION</u>

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The present invention is directed to the design and identification of modulators of protein tyrosine kinase function that are PTK subfamily specific, non-hydrolyzable under acidic conditions, and highly bioavailable. The three dimensional structures of a PTK optionally complexed with compounds can facilitate design and identification of modulators of PTK function.

Protein tyrosine kinases (PTKs) comprise a large and diverse class of enzymes. Schlessinger and Ullrich, 1992, Neuron 9: 383-391. The PTK family is subdivided into members that are receptors and those that are non-receptors. The PTK receptor family contains multiple subfamilies, one of which is the fibroblast growth factor receptor (FGF-R) PTK which is a molecule implicated in regulating angiogenesis a well as cellular proliferation and differentiation. Givol and Yayon, 1992, FASEB J. 6 (15): 3362-3369.

FGF-R1 can mediates cellular functions by its role in one or more cellular signal transduction processes. Cellular signal transduction processes comprise multiple steps that convert an extracellular signal into an

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intracellular signal.

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Receptor PTK mediated signal transduction is initiated by binding a specific extracellular ligand, followed by receptor dimerization, and subsequent autophosphorylation of the receptor PTK. The phosphate groups are binding sites for intracellular signal transduction molecules which leads to the formation of protein complexes at the cell membrane. These complexes facilitate an appropriate cellular effect (e.g., cell division, metabolic effects to the extracellular microenvironment) in response to the ligand that began the cascade of events.

Receptor PTKs function as binding sites for several intracellular proteins. Intracellular PTK binding proteins are divided into two principal groups: (1) 15 those which harbor a catalytic domain; and (2) those which lack such a domain but serve as adapters and associate with catalytically active molecules. Songyang et al., 1993, Cell 72:767-778. SH2 (src homology) 20 domains are common adaptors found in proteins which directly bind to the receptor PTK. SH2 domains are harbored by PTK binding proteins of both groups mentioned above. Fantl et al., 1992, Cell 69:413-423; Songyang et al., 1994, Mol. Cell. Biol. 14:2777-2785); 25 Songyang et al., 1993, Cell 72:767-778; and Koch et al., 1991, Science 252:668-678.

The specificity of the interactions between receptor PTKs and the SH2 domains of their binding proteins is determined by the amino acid residues immediately surrounding the phosphorylated tyrosine residue. Differences in the binding affinities of SH2

domains is correlated with the observed differences in substrate phosphorylation profiles of downstream molecules in the signal transduction process. Songyang et al., 1993, Cell 72:767-778. These observations suggest that the function of each receptor PTK is determined not only by its pattern of expression and ligand availability but also by the array of downstream signal transduction pathways that are activated by a particular receptor. Thus, PTKs provide a controlling regulatory role in signal transduction processes as a consequence of autophosphorylation.

PTK-mediated signal transduction regulates cell proliferative, differentiation, and metabolic responses in cells. Therefore, inappropriate PTK activity can result in a wide array of disorders and diseases. These disorders, which are described below, may be treated by the modulators of PTK function designed or identified by the methods disclosed herein.

The present invention also relates to crystalline polypeptides corresponding to the catalytic domain of receptor tyrosine kinases. Such tyrosine kinases include receptors of a class that are not covalently cross-linked but are understood to undergo ligand-induced dimerization, as well as cytoplasmic tyrosine kinases. Preferably, the crystalline catalytic domains are of sufficient quality to allow for the determination of a three-dimensional X-ray diffraction structure to a resolution of about 1.5 Å to about 2.5 Å. The invention also relates to methods for preparing and crystallizing the polypeptides. The polypeptides themselves, as well as information derived from their crystal structures can

be used to analyze and modify tyrosine kinase activity as well as to identify compounds that interact with the catalytic domain.

The polypeptides of the invention are designed on the basis of the structure of a region in the 5 cytoplasmic domain of the receptor tyrosine kinase that contains the catalytic domain. By way of illustration, FIG. 6A shows the amino acid sequence alignment of the catalytic domains of eighteen human receptor tyrosine 10 kinases; one representative member from each of the eighteen subfamilies is shown. FIG. 6B shows the alignment for cytoplasmic kinases. The applicants have discovered and determined the boundaries of the domain required for crystallization of the resulting 15 polypeptide. Surprisingly, these boundaries differ from that required for catalytic activity. For example, referring to FIG. 6A, the domain required for catalytic activity is generally believed to span about 7 amino acid residues upstream of the first glycine (FIG. 6A 20 residue number 485) of the N-terminal glycine-rich region through about 10 residues beyond the C-terminal conserved arginine (FIG. 6A, residue number 744). However, the additional sequence upstream of the Nterminal glycine-rich region and downstream of the C-25 terminal conserved arginine can be required for crystallization. In particular, at least about 20 amino acid residues (+/- 5 amino acid residues) upstream of the first glycine (i.e., FIG. 6A, residue number 485) in the conserved glycine-rich region of the catalytic 30 domain, and at least about 17 amino acid residues (+/- 5 amino acid residues) downstream of the conserved

arginine (<u>i.e.</u>, FIG. 6A, residue number 744) located at the C-terminal boundary of the catalytic domain can be required to engineer a polypeptide suitable for crystallization.

5 In those situations where the resulting polypeptide contains cysteine residues that interfere with crystallization (e.g., cysteine residue numbers 488 and 584 in the FGF-R1 sequence shown in FIG. 6A), such cysteine residues can be substituted with an appropriate 10 amino acid that does not readily form covalent bonds with other amino acid residues under crystallization conditions; e.g., by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non- β -stranded segment, based on secondary structure 15 assignments, are good candidates for replacement. For example, cysteines located in regions corresponding to the glycine-rich-loop, the kinase insert, the juxtamembrane region or the activation loop are prime candidates for replacement. However, substitutions of 20 cysteine residues that are conserved among the kinases (e.g., FIG. 6A at positions 725 and 736) are preferably avoided.

I. PTK Associated Diseases

Blood vessel proliferative disorders refer to angiogenic and vasculogenic disorders generally resulting in abnormal proliferation of blood vessels. The formation and spreading of blood vessels play important roles in a variety of physiological processes such as embryonic development, corpus luteum formation, wound healing and organ regeneration. They also play a

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pivotal role in cancer development. Other examples of blood vessel proliferation disorders include arthritis, where new capillary blood vessels invade the joint and destroy cartilage, and ocular diseases, like diabetic retinopathy, where new capillaries in the retina invade the vitreous, bleed and cause blindness. Conversely, disorders related to the shrinkage, contraction or closing of blood vessels are implicated in such diseases as restenosis.

10 Fibrotic disorders refer to the abnormal formation of extracellular matrix. Examples of fibrotic disorders include hepatic cirrhosis and mesangial cell proliferative disorders. Hepatic cirrhosis is characterized by the increase in extracellular matrix constituents resulting in the formation of a hepatic scar. Hepatic cirrhosis can cause diseases such as cirrhosis of the liver. An increased extracellular matrix resulting in a hepatic scar can also be caused by viral infection such as hepatitis.

Mesangial cell proliferative disorders refer to disorders brought about by abnormal proliferation of mesangial cells. Mesangial proliferative disorders include various human renal diseases, such as glomerulonephritis, diabetic nephropathy, malignant nephrosclerosis, thrombotic microangiopathy syndromes, transplant rejection, and glomerulopathies. The PDGF-R has been implicated in the maintenance of mesangial cell proliferation. Floege et al., 1993, Kidney International 43:475-545.

PTKs are directly associated with the cell proliferative disorders described above. For example,

some members of the receptor PTK family have been associated with the development of cancer. Some of these receptors, like EGFR (Tuzi et al., 1991, Br. J. Cancer 63:227-233; Torp et al., 1992, APMIS 100:713-5 719) HER2/neu (Slamon et al., 1989, Science 244:707-712) and PDGF-R (Kumabe et al., 1992, Oncogene 7:627-633) are over-expressed in many tumors and/or persistently activated by autocrine loops. In fact, PTK overexpression (Akbasak and Suner-Akbasak et al., 1992, J. Neurol. Sci. 111:119-133; Dickson et al., 1992, Cancer 10 Treatment Res. 61:249-273; Korc et al., 1992, J. Clin. Invest. 90:1352-1360) and autocrine loop stimulation (Lee and Donoghue, 1992, J. Cell. Biol. 118:1057-1070; Korc et al., supra; Akbasak and Suner-Akbasak et al., 15 supra) account for the most common and severe cancers. For example, EGFR is associated with squamous cell carcinoma, astrocytoma, glioblastoma, head and neck cancer, lung cancer and bladder cancer. HER2 is associated with breast, ovarian, gastric, lung, pancreas 20 and bladder cancer. PDGF-R is associated with glioblastoma, lung, ovarian, melanoma and prostate cancer. The receptor PTK c-met is generally associated with hepatocarcinogenesis and thus hepatocellular carcinoma. Additionally, c-met is linked to malignant 25 tumor formation. More specifically, c-met has been associated with, among other cancers, colorectal, thyroid, pancreatic and gastric carcinoma, leukemia and lymphoma. Additionally, over-expression of the c-met gene has been detected in patients with Hodgkins 30 disease, Burkitts disease, and the lymphoma cell line. The IGF-I receptor PTK, in addition to being

implicated in nutritional support and in type-II diabetes, is also associated with several types of cancers. For example, IGF-I has been implicated as an autocrine growth stimulator for several tumor types, 5 e.g. human breast cancer carcinoma cells (Arteaga et al., 1989, J. Clin. Invest. 84:1418-1423) and small lung tumor cells (Macauley et al., 1990, Cancer Res. 50:2511-2517). In addition, IGF-I, integrally involved in the normal growth and differentiation of the nervous system. 10 appears to be an autocrine stimulator of human gliomas. Sandberg-Nordqvist et al., 1993, Cancer Res. 53:2475-The importance of the IGF-IR and its modulators in cell proliferation is further supported by the fact that many cell types in culture (fibroblasts, epithelial 15 cells, smooth muscle cells, T-lymphocytes, myeloid cells, chondrocytes, osteoblasts, the stem cells of the bone marrow) are stimulated to grow by IGF-I. Goldring and Goldring, 1991, Eukaryotic Gene Expression 1:301-326. In a series of recent publications suggest that 20 IGF-IR plays a central role in the mechanisms of transformation and, as such, could be a preferred target for therapeutic interventions for a broad spectrum of human malignancies. Baserga, 1995, Cancer Res. 55:249-252; Baserqa, 1994, Cell 79:927-930; Coppola et al.. 1994, Mol. Cell. Biol. 14:4588-4595.

The association between abnormalities in receptor PTKs and disease are not restricted to cancer, however. For example, receptor PTKs are associated with metabolic diseases like psoriasis, diabetes mellitus, wound healing, inflammation, and neurodegenerative diseases. EGF-R is indicated in corneal and dermal wound healing.

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Defects in Insulin-R and IGF-IR are indicated in type-II diabetes mellitus. A more complete correlation between specific receptor PTKs and their therapeutic indications is set forth in Plowman et al., 1994, DN&P 7:334-339.

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Non-receptor PTKs, including src, abl, fps, yes, fyn, lyn, lck, blk, hck, fgr, yrk (reviewed by Bolen et al., 1992, FASEB J. 6:3403-3409), are involved in the proliferative and metabolic signal transduction pathways also associated with receptor PTKs. Therefore, the present invention is also directed towards designing modulators against this class of PTKs. For example, mutated src (v-src) is an oncoprotein (pp60^{v-src}) in chicken. Moreover, its cellular homolog, the protooncogene pp60c-src transmits oncogenic signals of many receptors. For example, over-expression of EGF-R or HER2/neu in tumors leads to the constitutive activation of pp60c-src, which is characteristic of the malignant cell but absent in the normal cell. On the other hand, mice deficient for the expression of c-src exhibit an osteopetrotic phenotype, indicating a key participation of c-src in osteoclast function and a possible involvement in related disorders. Similarly, Zap 70 is implicated in T-cell signaling. Both receptor PTKs and non-receptor PTKs are connected to hyperimmune disorders.

The instant invention is directed in part towards designing modulators of PTK function that could indirectly kill tumors by cutting off their source of sustenance. Normal vasculogenesis and angiogenesis play important roles in a variety of physiological processes such as embryonic development, wound healing, organ

regeneration and female reproductive processes such as follicle development in the corpus luteum during ovulation and placental growth after pregnancy. Folkman and Shing, 1992, J. Biological Chem. 267:10931-34.

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However, many diseases are driven by persistent unregulated or inappropriate angiogenesis. For example, in arthritis, new capillary blood vessels invade the joint and destroy the cartilage. In diabetes, new capillaries in the retina invade the vitreous, bleed and cause blindness. Folkman, 1987, in: Congress of Thrombosis and Haemostasis (Verstraete, et. al, eds.), Leuven University Press, Leuven, pp.583-596. Ocular neovascularization is the most common cause of blindness and dominates approximately twenty (20) eye diseases.

Moreover, vasculogenesis and/or angiogenesis can be associated with the growth of malignant solid tumors and metastasis. A tumor must continuously stimulate the growth of new capillary blood vessels for the tumor itself to grow. Furthermore, the new blood vessels embedded in a tumor provide a gateway for tumor cells to enter the circulation and to metastasize to distant sites in the body. Folkman, 1990, J. Natl. Cancer Inst. 82:4-6; Klagsbrunn and Soker, 1993, Current Biology 3:699-702; Folkman, 1991, J. Natl., Cancer Inst. 82:4-6; Weidner et al., 1991, New Engl. J. Med. 324:1-5.

Several polypeptides with in vitro endothelial cell growth promoting activity have been identified. Examples include acidic and basic fibroblastic growth factor (α FGF, β FGF), vascular endothelial growth factor (VEGF) and placental growth factor. Unlike α FGF and β FGF, VEGF has recently been reported to be an

endothelial cell specific mitogen. Ferrara and Henzel, 1989, Biochem. Biophys. Res. Comm. 161:851-858; Vaisman et al., 1990, J. Biol. Chem. 265:19461-19566.

Thus, identifying the specific receptors that bind

FGF or VEGF is important for understanding endothelial cell proliferation regulation. Two structurally related receptor PTKs that bind VEGF with high affinity are identified: the flt-1 receptor (Shibuya et al., 1990, Oncogene 5:519-524; De Vries et al., 1992, Science

255:989-991) and the KDR/FLK-1 receptor, discussed in the U.S. Patent Application No. 08/193,829. In addition, a receptor that binds αFGF and βFGF is identified. Jaye et al., 1992, Biochem. Biophys. Acta 1135:185-199). Consequently, these receptor PTKs most likely regulate endothelial cell proliferation.

FGFRs play important roles in angiogenesis, wound healing, embryonic development, and malignant transformation. Basilico and Moscatelli, 1992, Adv. Cancer Res. 59:115-165. Four mammalian FGFR (FGFR1-4) have been described and additional diversity is generated by alternative RNA splicing within the extracellular domains. Jaye et al., 1992, Biochem. Biophys. Acta 1135:185-199. Like other receptor PTKs, dimerization of FGF receptors is essential for their activation. Soluble or cell surface-bound heparin sulfate proteoglycans act in concert with FGF to induce dimerization (Schlessinger et al., 1995, Cell 83:357-360), which leads to autophosphorylation of specific tyrosine residues in the cytoplasmic domain. Mohammadi et al., 1996, Mol. Cell Biol. 16:977-989.

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Mutations in three human FGF receptor genes, FGFR1,

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FGFR2, and FGFR3, have been implicated in a variety of human genetic skeletal disorders. Mutations in FGFR1 and FGFR2 result in the premature fusion of the flat bones of the skull and cause the craniosynostosis syndromes, such as Apert (FGFR2) (Wilkie et al., 1994, Nat. Genet. 8:269-274), Pfeiffer (FGFR1 and FGFR2) (Muenke et al., 1994, Nat. Genet. 8:269-274), Jackson-Weiss (FGFR2) (Jabs et al., 1994, Nat. Genet. 8:275-279) and Crouzon (FGFR2) (Jabs et al., 1994, Nat. Genet. 8:275-279) syndromes. In contrast mutations in FGFR3 are implicated in long bone disorders and cause several clinically related forms of dwarfism including achondroplasia (Shiang et al., 1994, Cell 78:335-342), hypochondroplasia (Bellus et al., 1995, Nat. Genet. 10:357-359) and the neonatal lethal thanatophoric dysplasia (Tavormina et al., 1995, Nat. Genet. 9:321-328). It has been shown that these mutations lead to constitutive activation of the tyrosine kinase activity of FGFR3 (Webster et al., 1996, EMBO J. 15:520-527). Furthermore gene-targeting experiments in mice have revealed an essential role for FGFR3 in developmental

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Another major role proposed for FGFs in vivo is the induction of angiogenesis (Folkman and Klagsbrun, 1987, Science 236:442). Therefore, inappropriate expression of FGFs or of their receptors or aberrant function of the tyrosine kinase activity could contribute to several human angiogenic pathologies such as diabetic retinopathy, rheumatoid arthritis, atherosclerosis and tumor neovascularization (Klagsbrun and Edelman, 1989, Arteriosclerosis 9:269). Moreover, FGFs are thought to

bone formation (Deng et al., 1996, Cell 84:911-921).

be involved in malignant transformation. Indeed, the genes coding for the three FGF homologues int-2, FGF-5 and hst-1/K-fgf were originally isolated as oncogenes. Furthermore, the cDNA encoding FGFR1 and FGFR2 are amplified in a population of breast cancers (Adnane et al., 1991, Oncogene 6:659-663). Over-expression of FGF receptors has been also detected in human pancreatic cancers, astrocytomas, salivary gland adenosarcomas, Kaposi sarcomas, ovarian cancers and prostate cancers.

Evidence, such as the disclosure set forth in copending U.S. Application Serial No. 08/193,829, strongly suggests that VEGF is not only responsible for endothelial cell proliferation, but also is a prime regulator of normal and pathological angiogenesis. See generally, Klagsburn and Soker, 1993, Current Biology 3:699-702; Houck et al., 1992, J. Biol. Chem. 267:26031-26037. Moreover, it has been shown that KDR/FLK-1 and flt-1 are abundantly expressed in the proliferating endothelial cells of a growing tumor, but not in the surrounding quiescent endothelial cells. Plate et al., 1992, Nature 359:845-848; Shweiki et al., 1992, Nature 359:843-845.

The invention is directed to designing and identifying modulators of receptor and non-receptor PTK functions that could modify the inappropriate activity of a PTK involved with a clinical disorder. The rational design and identification of modulators of PTK functions can be accomplished by utilizing the structural coordinates that define a PTK three dimensional structure.

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II. <u>Modulators of PTK functions as Therapeutics for Disease</u>

As a consequence of the disorders discussed above, scientists in the biomedical community are searching for modulators of PTK functions that down-regulate signal transduction pathways associated with inappropriate PTK activity.

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functions are sought as some can traverse the cell
membrane and do not hydrolyze in acidic environments.
Some compounds have already been discovered. For
example, bis monocyclic, bicyclic or heterocyclic aryl
compounds (PCT WO 92/20642), vinylene-azaindole
derivatives (PCT WO 94/14808) 1-cyclopropyl-4-pyridylquinolones (U.S. Patent No. 5,330,992), styryl compounds
(U.S. Patent No. 5,217,999), styryl-substituted pyridyl
compounds (U.S. Patent No. 5,302,606), certain
quinazoline derivatives (EP Application No. 0 566 266
Al), seleoindoles and selenides (PCT WO 94/03427),
tricyclic polyhydroxylic compounds (PCT WO 92/21660),
and benzylphosphonic acid compounds (PCT WO 91/15495)
are described as PTK inhibitors.

Although some modulators of PTK function are known, many of these are not specific for PTK subfamilies and

will therefore cause multiple side-effects as therapeutics. Compounds of the oxindolinone/
thiolindolinone family, however, are specific for the FGF receptor subfamily (U.S. Patent Application Serial No. 08/702,232, filed August 23, 1996, invented by Tang et al., entitled "Indolinone Combinatorial Libraries and Related Products and Methods for the Treatment of

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Disease," Attorney Docket No. 221/187). In addition, compounds of the oxindolinone/thiolindolinone family are non-hydrolyzable in acidic conditions and can be highly bioavailable.

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5 The invention provides information regarding the specific interactions between a PTK and compounds of the oxindolinone/thiolindolinone family. Although the use of X-ray crystallography has provided three dimensional structures of other PTKs, the PTKs in these structures 10 are not complexed with PTK subfamily specific, hydrolysis resistant, highly bioavailable small molecules. The X-ray crystallography techniques used in the current invention resolve interactions between a PTK and compounds in complex with it at the atomic level, 15 which provides detailed information regarding the orientation of chemical groups defining an effective modulator of PTK function.

III. Crystalline Tyrosine Kinases

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20 Crystalline PTKs of the invention include native crystals, derivative crystals and co-crystals. The native crystals of the invention generally comprise substantially pure polypeptides corresponding to the tyrosine kinase domain in crystalline form.

It is to be understood that the crystalline tyrosine kinase domains of the invention are not limited to naturally occurring or native tyrosine kinase domains. Indeed, the crystals of the invention include mutants of native tyrosine kinase domains. Mutants of native tyrosine kinase domains are obtained by replacing at least one amino acid residue in a native tyrosine

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kinase domain with a different amino acid residue, or by adding or deleting amino acid residues within the native polypeptide or at the N- or C-terminus of the native polypeptide, and have substantially the same three-dimensional structure as the native tyrosine kinase domain from which the mutant is derived.

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By having substantially the same three-dimensional structure is meant having a set of atomic structure coordinates that have a root-mean-square deviation of less than or equal to about 2Å when superimposed with the atomic structure coordinates of the native tyrosine kinase domain from which the mutant is derived when at least about 50% to 100% of the C α atoms of the native tyrosine kinase domain are included in the superposition.

Amino acid substitutions, deletions and additions which do not significantly interfere with the three-dimensional structure of the tyrosine kinase domain will depend, in part, on the region of the tyrosine kinase domain where the substitution, addition or deletion occurs. In highly variable regions of the molecule, such as those shown in FIG. 6, non-conservative substitutions as well as conservative substitutions may be tolerated without significantly disrupting the three-dimensional structure of the molecule. In highly conserved regions, or regions containing significant secondary structure, such as those regions shown in FIG. 6, conservative amino acid substitutions are preferred.

Conservative amino acid substitutions are wellknown in the art, and include substitutions made on the basis of similarity in polarity, charge, solubility,

hydrophobicity, hydrophilicity and/or the amphipathic nature of the amino acid residues involved. For example, negatively charged amino acids include aspartic acid and glutamic acid; positively charged amino acids include lysine and arginine; amino acids with uncharged polar head groups having similar hydrophilicity values include the following: leucine, isoleucine, valine; glycine, alanine; asparagine, glutamine; serine, threonine; phenylalanine, tyrosine. Other conservative amino acid substitutions are well known in the art.

For tyrosine kinase domains obtained in whole or in part by chemical synthesis, the selection of amino acids available for substitution or addition is not limited to the genetically encoded amino acids. Indeed, the mutants described herein may contain non-genetically encoded amino acids. Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete and/or add amino acid residues to a native tyrosine kinase domain in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the polypeptide, and for crystallization of the polypeptide. Such substitutions, deletions and/or additions which do not substantially alter the three dimensional structure of the native tyrosine kinase

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domain will be apparent to those of ordinary skill in the art.

It should be noted that the mutants contemplated herein need not exhibit PTK activity. Indeed, amino acid substitutions, additions or deletions that interfere with the kinase activity of the tyrosine kinase domain but which do not significantly alter the three-dimensional structure of the domain are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to identify compounds that bind to the native domain. These compounds may affect the activity or the native domain.

The derivative crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in covalent association with one or more heavy metal atoms. The polypeptide may correspond to a native or a mutated tyrosine kinase domain. Heavy metal atoms useful for providing derivative crystals include, by way of example and not limitation, gold, mercury, etc.

The co-crystals of the invention generally comprise a crystalline tyrosine kinase domain polypeptide in association with one or more compounds. The association may be covalent or non-covalent. Such compounds include, but are not limited to, cofactors, substrates, substrate analogues, inhibitors, allosteric effectors, etc.

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IV. Three Dimensional Structure Determination Using X-ray Crystallography

X-ray crystallography is a method of solving the three dimensional structures of molecules. The structure of a molecule is calculated from X-ray diffraction patterns using a crystal as a diffraction grating. Three dimensional structures of protein molecules arise from crystals grown from a concentrated aqueous solution of that protein. The process of X-ray crystallography can include the following steps:

- (a) synthesizing and isolating a polypeptide;
- (b) growing a crystal from an aqueous solution comprising the polypeptide with or without a modulator; and
- (c) collecting X-ray diffraction patterns from the crystals, determining unit cell dimensions and symmetry, determining electron density, fitting the amino acid sequence of the polypeptide to the electron density, and refining the structure.

Production of Polypeptides

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polypeptides described herein may be chemically synthesized in whole or part using techniques that are well-known in the art (see, e.g., Creighton, 1983).

Alternatively, methods which are well known to those skilled in the art can be used to construct expression vectors containing the native or mutated tyrosine kinase domain polypeptide coding sequence and appropriate

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transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques and *in vivo* recombination/genetic recombination. See, for example, the techniques described in Maniatis et al., 1989 and Ausubel et al., 1989.

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A variety of host-expression vector systems may be utilized to express the tyrosine kinase domain coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing the tyrosine kinase domain coding sequence; yeast transformed with recombinant yeast expression vectors containing the tyrosine kinase domain coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing the tyrosine kinase domain coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing the tyrosine kinase domain coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, may be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of bacteriophage λ , plac, ptrp,

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ptac (ptrp-lac hybrid promoter) and the like may be used; when cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter may be used; when cloning in plant cell systems, promoters derived 5 from the genome of plant cells (e.g., heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) may 10 be used; when cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) may be used; when 15 generating cell lines that contain multiple copies of the tyrosine kinase domain DNA, SV40-, BPV- and EBVbased vectors may be used with an appropriate selectable marker.

vectors, various types of cells used, methods of incorporating the vectors into the cells, expression techniques, protein purification and isolation methods, and protein concentration methods are disclosed in detail with respect to the protein PYK-2 in PCT publication WO 96/18738. This publication is incorporated herein by reference in its entirety, including any drawings. Those skilled in the art will appreciate that such descriptions are applicable to the present invention and can be easily adapted to it.

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Crystal Growth

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Crystals are grown from an aqueous solution containing the purified and concentrated polypeptide by a variety of techniques. These techniques include batch, liquid, bridge, dialysis, vapor diffusion, and hanging drop methods. McPherson, 1982, John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189:1-23; Webber, 1991, Adv. Protein Chem. 41:1-36, incorporated by reference herein in its entirety, including all figures, tables, and drawings.

Generally, the native crystals of the invention are grown by adding precipitants to the concentrated solution of the polypeptide corresponding to the PTK catalytic domain. The precipitants are added at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

For crystals of the invention, it has been found that hanging drops containing about 2.0 μ L of tyrosine kinase domain polypeptide (10 mg/mL in 10mM Tris-HCl, pH 8.0, 10 mM NaCl and 2 mM dithiothreitol) and 2.0 μ L reservoir solution (16% w/v polyethylene glycol MW 10000, 0.3 M (NH₄)₂SO₄, 5% v/v ethylene glycol or glycerol and 100 mM bis-Tris, pH 6.5) suspended over 0.5 mL reservoir buffer for about 3-4 weeks at 4°C provide crystals suitable for high resolution X-ray structure determination.

Those of ordinary skill in the art will recognize that the above-described crystallization conditions can be varied. Such variations may be used alone or in

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combination, and include polypeptide solutions containing polypeptide concentrations between about 1 mg/mL and about 60 mg/mL, Tris-HCl concentrations between about 10 mM and about 200 mM, dithiothreitol concentrations between about 0 mM and about 20 mM, pH ranges between about 5.5 and about 7.5; and reservoir solutions containing polyethylene glycol concentrations between about 10% and about 30% (w/v), polyethylene glycol molecular weights between about 1000 and about 20,000, (NH₄)₂SO₄ concentrations between about 0.1 M and about 0.5 M, ethylene glycol or glycerol concentrations between about 0% and about 20% (v/v), bis-Tris concentrations between about 10 mM and about 200 mM, pH ranges between about 5.5 and about 7.5 and temperature ranges between about 0°C and about 25°C. Other buffer solutions may be used such as HEPES buffer, so long as the desired pH range is maintained.

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Derivative crystals of the invention can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. It has been found that soaking a native crystal in a solution containing about 0.1 mM to about 5 mM thimerosal, 4-chloromeruribenzoic acid or KAu(CN)₂ for about 2 hr to about 72 hr provides derivative crystals suitable for use as isomorphous replacements in determining the X-ray crystal structure of the tyrosine kinase domain polypeptide.

Co-crystals of the invention can be obtained by soaking a native crystal in mother liquor containing compound that bind the kinase domain, or described above, or can be obtained by co-crystallizing the kinase

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domain polypeptide in the presence of one or more binding compounds.

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For co-crystals of tyrosine kinase domain polypeptide in co-complex with AMP-PCP, it has been found that co-crystallizing the kinase domain polypeptide in the presence of AMP-PCP using the abovedescribed crystallization conditions for obtaining native crystals with a polypeptide solution additionally containing 10 mM AMP-PCP and 20 mM MqCl, yields cocrystals suitable for the high resolution structure determination by X-ray crystallography. Of course, those having skill in the art will recognize that the concentrations of AMP-PCP and MqCl₂ in the polypeptide solution can be varied, alone or in combination with the variations described above for native crystals. Such variations include polypeptide solutions containing AMP-PCP concentrations between 0.1 mM and 50 mM and MgCl₂ concentrations between 0 mM and 50 mM.

20 a PTK catalytic domain complexed with a compound can be grown by one of two methods. In the first method, the modulator is added to the aqueous solution containing the polypeptide corresponding to the PTK catalytic domain before the crystal is grown. In the second

25 method, the modulator is soaked into an already existing crystal of a polypeptide corresponding to a PTK catalytic domain.

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Crystalline FGFR

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In one illustrative embodiment, the invention provides crystals of FGFR1. The crystals were obtained by the methods provided in the Examples. The FGFR1 crystals, which may be native crystals, derivative crystals or co-crystals, have monoclinic unit cells (i.e., unit cells wherein $a\neq b\neq c$; $\alpha=\gamma=90^{\circ}$; and $\beta>90^{\circ}$) and space group symmetry C2. There are two FGFR1 molecules in the asymmetric unit, related by an approximate two-fold axis.

Two forms of crystalline FGFR1 were obtained. In one form (designated "C2-A form"), the unit cell has dimensions of a=208.3 Å, b=57.2 Å, c=65.5 Å and β =107.2°. In another form (designated "C2-B form"), the unit cell has dimensions of a=211.6 Å, b=51.3 Å, c=66.1 Å and β =107.7°.

Three distinct two-fold related FGFR1 dimers are observed in both the C2-A and C2-B forms of the FGFR1 crystal, one non-crystallographically related dimer and two crystallographically related dimers. The non-crystallographically related dimer comprises the two molecules in the asymmetric unit. The residues making up the dimer interface are located in C-terminal lobe. In this dimer, the C-terminal lobes abut with the N-terminal lobes distal to one another. The total amount of surface area buried in the surface is about 950 Ų. Very few of the interactions in the interface are of a specific nature, e.g., hydrogen-bonding or close packing of hydrophobic residues.

There are two crystallographically-related dimers in the C2 lattice. In the first dimer, the residues

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that constitute the dimer interface are limited to those in the β -sheet of the N-terminal lobe (amino acid residues 477, 479, 498, 506, 508 and 496). The total surface area buried in this interface is about 670 Å2. The interactions are rather specific. Three hydrophobic residues which are partially solvent-exposed in the monomer, Val-479, Ile-498 and Val-508, come together with their two-fold-related residues to form a compact hydrophobic plug. This plug is capped on either side by a salt bridge between Arg-477 and Glu-496. In addition. two main-chain hydrogen-bonds connect the β-sheets of the two monomers at the start of \$3 (amino acid residues 506 and 508). The residues in this dimer interface, or their residue character, are generally conserved in the mammalian FGF receptors, but not in the invertebrate homologues.

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The other crystallographically-related dimer buries about 1650 ${\rm \AA}^2$ in its interface. In this dimer, the αC helices of the two monomers are nearly parallel and contact each other at their C-terminal ends. Met-534 and Met-537 are in van der Waals contact with their two-fold-related residues. Other hydrophobic contacts involve Pro-466 with Ile-648 and Pro-469 with Ile-676 and Thr-678. In addition, hydrogen bonds (side-chain to main-chain) are made between Arg-470 and Lys-618 and between His-649 and Glu-464, and there are several water molecules that bridge the two monomers through hydrogen bonding.

In the C2-B form of the crystal, the monomers of this second crystallographically-related dimer are shifted slightly with respect to one another (6°

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rotation), indicating that this interface is somewhat fluid.

In both of the crystallographically-related dimers, the N-termini of the two molecules comprising the dimer point in the same direction and are reasonably close to one another.

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Determining Unit Cell Dimensions and the Three Dimensional Structure of a Polypeptide or Polypeptide Complex

Once the crystal is grown, it can be placed in a glass capillary tube and mounted onto a holding device connected to an X-ray generator and an X-ray detection device. Collection of X-ray diffraction patterns are well documented by those in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. A beam of X-rays enter the crystal and then diffract from the crystal. An X-ray detection device can be utilized to record the diffraction patterns emanating from the crystal. Although the X-ray detection device on older models of these instruments is a piece of film, modern instruments digitally record X-ray diffraction scattering.

25 Methods for obtaining the three dimensional structure of the crystalline form of a peptide molecule or molecule complex are well known in the art. Ducruix and Geige, 1992, IRL Press, Oxford, England, and references cited therein. The following are steps in the process of determining the three dimensional structure of a molecule or complex from X-ray diffraction data.

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After the X-ray diffraction patterns are collected from the crystal, the unit cell dimensions and orientation in the crystal can be determined. They can be determined from the spacing between the diffraction emissions as well as the patterns made from these emissions. The unit cell dimensions are characterized in three dimensions in units of Angstroms (one $\dot{A}=10^{-10}$ meters) and by angles at each vertices. The symmetry of the unit cell in the crystals is also characterized at this stage. The symmetry of the unit cell in the crystal simplifies the complexity of the collected data by identifying repeating patterns. Application of the symmetry and dimensions of the unit cell is described below.

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Each diffraction pattern emission is characterized as a vector and the data collected at this stage of the method determines the amplitude of each vector. phases of the vectors can be determined using multiple techniques. In one method, heavy atoms can be soaked into a crystal, a method called isomorphous replacement, and the phases of the vectors can be determined by using these heavy atoms as reference points in the X-ray analysis. Otwinowski, 1991, Daresbury, United Kingdom, 80-86. The isomorphous replacement method usually requires more than one heavy atom derivative. another method, the amplitudes and phases of vectors from a crystalline polypeptide with an already determined structure can be applied to the amplitudes of the vectors from a crystalline polypeptide of unknown structure and consequently determine the phases of these vectors. This second method is known as molecular

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replacement and the protein structure which is used as a reference must have a closely related structure to the protein of interest. Naraza, 1994, Proteins 11:281-296. Thus, the vector information from a PTK of known structure, such as those reported herein, are useful for the molecular replacement analysis of another PTK with unknown structure.

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Once the phases of the vectors describing the unit cell of a crystal are determined, the vector amplitudes and phases, unit cell dimensions, and unit cell symmetry can be used as terms in a Fourier transform function. The Fourier transform function calculates the electron density in the unit cell from these measurements. electron density that describes one of the molecules or one of the molecule complexes in the unit cell can be referred to as an electron density map. The amino acid structures of the sequence or the molecular structures of compounds complexed with the crystalline polypeptide may then fit to the electron density using a variety of computer programs. This step of the process is sometimes referred to as model building and can be accomplished by using computer programs such as TOM/FRODO. Jones, 1985, Methods in Enzymology 115:157-171.

A theoretical electron density map can then be calculated from the amino acid structures fit to the experimentally determined electron density. The theoretical and experimental electron density maps can be compared to one another and the agreement between these two maps can be described by a parameter called an R-factor. A low value for an R-factor describes a high

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degree of overlapping electron density between a theoretical and experimental electron density map.

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The R-factor is then minimized by using computer programs that refine the theoretical electron density map. A computer program such as X-PLOR can be used for model refinement by those skilled in the art. Brünger, 1992, Nature 355:472-475. Refinement may be achieved in an iterative process. A first step can entail altering the conformation of atoms defined in an electron density map. The conformations of the atoms can be altered by simulating a rise in temperature which will increase the vibrational frequency of the bonds and modify positions of atoms in the structure. At a particular point in the atomic perturbation process, a force field, which typically defines interactions between atoms in terms of allowed bond angles and bond lengths, Van der Waals interactions, hydrogen bonds, ionic interactions, and hydrophobic interactions, can be applied to the system of atoms. Favorable interactions may be described in terms of free energy and the atoms can be moved over many iterations until a free energy minimum is achieved. The refinement process can be iterated until the Rfactor reaches a minimum value.

The three dimensional structure of the molecule or molecule complex is described by atoms that fit the theoretical electron density characterized by a minimum R-value. A file can then be created for the three dimensional structure that defines each atom by coordinates in three dimensions. Examples of such structural coordinate files are defined in Table 1, Table 2, Table 3, and Table 4.

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V. Structures of FGFR1

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The present invention provides high-resolution three-dimensional structures and atomic structure coordinates of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the examples. The atomic structure coordinates of crystalline FGFR1, obtained from the C2-A form of the crystal to 2.0 Å resolution, are listed in Table 3; the coordinates of crystalline FGFR1:AMP-PCP co-complex, obtained from the C2-A form of the crystal to 2.3 Å resolution are listed in Table 4.

Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of FGFR1, whether native crystals, derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 1.5 Å when superimposed, using backbone atoms (N, C_{α} , C and O), on the structure coordinates listed in Table 3 or Table 4 are considered to be identical with the structure coordinates listed in the Tables when at least about 50% to 100% of the backbone atoms of FGFR1 are included in the superposition.

Referring now to FIG. 1, the overall structure of FGFR1 is bi-lobate. The N-terminal lobe of FGFR1 spans amino acid residues 456-567 (FIG. 3) and comprises a curled β -sheet of five anti-parallel strands (β 1- β 5) and

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one α -helix (α C). The C-terminal lobe spans amino acid residues 568-765 (FIG. 3) and comprises two β -strands (β 7, β 8) and seven α -helices (α D, α E, α EF, α F- α I). The secondary structure nomenclature follows that used for IRK (Hubbard et al., 1994) which in turn is based on the assignments for cAPK (Knighton et al., 1991). FIG. 2 shows a stereo view of a C_{α} trace of FGFR1 in the same orientation as FIG. 1.

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A structure-based sequence alignment of the tyrosine kinase domains of human fibroblast growth 10 factor receptor 1 (human FGFR1; labelled FGFR1), human fibroblast growth factor receptors 2, 3 and 4 (labelled FGFR2, FGFR3 and FGFR4, respectively), a D. melanogaster homologue (labelled DFDFR1), a C elegans homologue 15 (labelled EGL-15) and insulin receptor kinase (labelled IRK), is shown in FIG. 3. The sequence of FGFR1, which is not shown in FIG. 3 is identical to the sequence of FGFR1 except that FGFR1 has the following amino acid substitutions and additions: Cys-488 - Ala, Cys-584 -20 Ser, Leu-457 → Val and an additional five N-terminal amino acids (Ser-Ala-Ala-Gly-Thr). The secondary structure assignments for FGFR1 and IRK were obtained using the Kabsch and Sander algorithm (Kabsch and Sander, 1983) as implemented in PROCHECK (Laskowski et 25 al., 1993). In the FGF receptor sequences, a period represents sequence identity to FGFR1. In the IRK sequence, residues that are identical to FGFR1 are highlighted. A hyphen denotes an insertion.

The numbers under the EGL-15 sequence represent the fractional solvent accessibility (FSA2) of the residue in the FGFR1 structure. The FSA ratio is the ratio of

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the solvent-accessible surface area of a residue in a Gly-X-Gly tripeptide compared to that in the FGFR1 structure. A value of 0 represents an FSA between 0.00 and 0.09; 1 represents an FSA between 0.10 and 0.19, etc. The higher the value, the more solvent-exposed the residue. An asterisk or pound sign in the FSA line indicates that the residue (asterisk) or side chain (pound sign) is not included in the atom model due to disorder. The numbers below the FSA line are the FSAs for those residues that form part of a dimer interface.

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The amino acid residue numbers for FGFR1, and hence FGFR1, and IRK provided in FIG. 3 are used in the discussion that follows. Significant differences in the N-terminal lobe of FGFR1 as compared to IRK are found in the loops between β strands and in $\alpha C.$ Residues from the end of $\beta1$ through the beginning of $\beta2$ (amino acid residues 485-490) form the nucleotide-binding loop, named because of its role in ATP coordination. residue stretch contains the protein kinase-conserved GXGXXG sequence motif, where X is any amino acid. This loop is poorly ordered in one FGFR1 molecule in the asymmetric unit and disordered (i.e., not included in the atomic model) in the other FGFR1 molecule in the asymmetric unit. The loop between $\beta1$ and $\beta3$ is disordered in both FGFR1 molecules comprising the asymmetric unit.

Referring now to FIG. 4A, which provides a ribbon diagram of the N-terminal lobes of FGFR1 and IRK in which the C_{α} atoms of the β -sheets have been superimposed, it can be seen that in FGFR1 αC is longer by one helical turn than in IRK and is oriented such

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that residues Lys-514 and Glu-531, which are conserved in protein kinases, form a salt bridge (represented by a black line). While not intending to be bound by theory, this salt bridge is believed to be important for proper positioning of the conserved lysine side chain, which coordinates two phosphate oxygens of ATP. The salt bridge is observed in the structures of cAPK (Knighton et al., 1991) and mitogen-activated protein kinase (MAPK) (Zhang et al., 1994).

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Referring now to FIG. 4B, which provides a ribbon diagram of the C-terminal lobes of FGFR1 and IRK in which the C_{α} atoms of the α -helices have been superimposed, a significant difference is found in the C-terminal helix of FGFR1 when compared to IRK; helix α I of FGFR1 is longer by seven residues (two helical turns) than its counterpart in IRK. The extended length of α I is presumably important in the biological functioning of FGF receptors, since the tyrosine autophosphorylation site to which an SH2 domain of PLCy binds is six residues C-terminal to this helix.

The structure of FGFR1 displays an open disposition of the N- and C-terminal lobes. Despite having different sets of lattice contacts, the two FGFR1 molecules in the asymmetric unit have only a 2° difference in relative lobe orientation. It appears as though the stearic interaction between residues in α C (Glu-531 and Met-534) with Phe-642 and Gly-643 of the protein kinase-conserved DFG sequence at the beginning of the activation loop accounts for the open conformation of FGFR1.

The active site of FGFR1 is characterized by at

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least amino acid residues spanning the catalytic loop, activation loop and nucleotide binding loop. Unlike the structure of IRK, in which Tyr-1162 occupies the active site of the molecule, the active sites of both FGFR1 molecules in the asymmetric unit are unoccupied.

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The activation loop, which regulates phosphorylation, is characterized by at least resides 640 to 663. Quite surprisingly, while the activation loops of FGFR1 and IRK contain the same number of amino acid residues and share greater than 50% sequence homology, the paths of the polypeptide chains are strikingly dissimilar, diverging at Ala-640 (Gly-1149 in IRK) and reconverging at Val-664 (Val-1173 in IRK). Tyr-653 and Tyr 564 are not bound in the active site. Instead, these residues point away from it. Tyr-653 is in van der Waals contact with several hydrophobic residues (Val-664, Leu-672 and Phe-710) and is hydrogenbonded via its hydroxyl group to a backbone carbonyl oxygen (Leu-672). Tyr-654 is more solvent exposed than Tyr-653, and its only van der Waals contact is with Val-Temperature factor data suggest that the activation loop is relatively mobile and adopts multiple conformations.

The catalytic loop of protein kinases lies between secondary structure elements αE and $\beta 7$ and contains an invariant aspartic acid residue (Asp-623 in FGFR1) which serves as the catalytic base in the phosphotransfer reaction, abstracting the proton from the hydroxyl group of the substrate tyrosine, serine or threonine. The catalytic loop sequence of FGFR1 comprises at least residues His-621 to Asn-628 (amino acid sequence

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HRDLAARN), and is identical to that for IRK and most receptor and non-receptor PTKs.

In addition to the two tyrosine autophosphorylation sites in the activation loop (Tyr-653 and Tyr-654),

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10 varying degrees of conservation in mammalian FGF receptors: Tyr-463 and Tyr-585 in FGFR1 and 2; Tyr-583 in FGFR1, 2 and 3; and Tyr-730 in FGFR 1, 2, 3 and 4 (FIG. 3).

Referring now to FIG. 5, the positions of the autophosphorylation sites are mapped onto the FGFR1 structure. The juxtamembrane site (Tyr-463) and the residues N-terminal to it are disordered in one of the FGFR1 molecules in the asymmetric unit. In the other molecule in the asymmetric unit Tyr-463 is involved in a lattice contact.

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The kinase insert region (the region between helices αD and αE) contains autophosphorylation sites Tyr-583 and Tyr-585 and is disordered in both FGFR1 molecules in the asymmetric unit of the C2-A form of the crystal. In the C2-B form, several lattice contacts partially pin down this region in one of the two FGFR1 molecules in the asymmetric unit, allowing a trace of the polypeptide chain to be made. There is no well-defined secondary structure for these residues. Tyr-730, situated in αH in the C-terminal lobe, is nearly buried and the side-chain hydroxyl group makes two

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hydrogen-bonds. The side chains of neighboring Met-732 and Met-733 are both buried. Therefore, phosphorylation of Tyr-730 would presumably require prior unfolding of α H.

Aside from Tyr-730, the five other
autophosphorylation sites (including Tyr-653 and Tyr654) are found in relatively mobile segments of the
FGFR1 molecule. While not intending to be bound by
theory, the spatial positions of the autophosphorylation
sites relative to the active site suggest that
autophosphorylation occurs by a trans mechanism between
two kinase domains, supporting the hypothesis that
ligand-induced receptor dimerization is critical for the
initiation of autophosphorylation events.

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The structure of crystalline FGFR1:AMP-PCP cocomplex is essentially similar to that observed for crystalline FGFR1. There are no significant changes in the structure of FGFR1 induced by AMP-PCP binding. In particular, binding of AMP-PCP, and by extension ATP, does not by itself promote lobe closure under the crystallization conditions used. Furthermore, complexation did not result in any noticeable changes in the conformations of the activation and nucleotide-binding loops.

The crystalline FGFR1:AMP-PCP co-complex contains hydrogen bonds that are present between N1 of adenine and the amide nitrogen of Ala-564 and between N6 of adenine and the carbonyl oxygen of Glu-562. The adenine ring is flanked on one side by Leu-484 and Val-492 (N-terminal lobe) and on the other side by Leu-630 (C-terminal lobe). The ribose hydroxyl groups make no

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direct hydrogen bonds with protein atoms. Lys-514 is hydrogen-bonded to oxygens of the β - and γ -phosphates. There is no unambiguous electron density that would indicate the positions of Mg² ions. Generally, AMP-PCP appears to be coordinated rather loosely to unphosphorylated FGFR1, being bound to the "roof" of the cleft rather than being tightly sandwiched between the two kinase lobes.

10 Structural Differences Between FGF-R and IRK

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Several features distinguish the FGF-receptor structure from that of the insulin-receptor tyrosine kinase. These distinctions are likely to be important in signaling by FGF-receptors, and other monomeric receptors that are believed to undergo ligand-induced dimerization.

The most significant difference between the structures of FGFR1 and IRK is the conformation of the activation loop. In FGFR1, the activation loop is disposed such that the binding site for substrate peptides is blocked not by an activation loop tyrosine, as in IRK, but by Arg-661 and PTK-invariant Pro-663, while the ATP binding site is accessible. This represents another molecular mechanism by which a receptor PTK may be autoinhibited. The observed autoinhibition in FGFR1 would appear to be weaker than that in IRK because of fewer specific interactions made by residues in the FGFR1 activation loop (manifested in the relatively higher B-values) and the accessibility of the ATP site. One obvious distinction between the insulin and FGF receptor families is that in the former,

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receptors are covalently linked heterotetramers $(\alpha_2\beta_2)$, whereas in the latter, receptor dimerization is ligand dependent. Receptors whose kinase domains are always in close proximity may require a stronger autoinhibition mechanism than those receptors that associate only upon ligand binding (Taylor et al., 1995). Since most growth factor receptors undergo ligand-dependent dimerization and activation, the FGF receptor autoinhibition mechanism appears to be a more general one.

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VI. Uses of the Crystals and Atomic Structure Coordinates

The crystals of the invention, and particularly the atomic structure coordinates obtained therefrom, have a wide variety of uses. For example, the crystals described herein can be used as a starting material in any of the art-known methods of use for receptor and non-receptor tyrosine kinases. Such methods of use include, for example, identifying molecules that bind to the native or mutated catalytic domain of tyrosine kinases. The crystals and structure coordinates are particularly useful for identifying compounds that inhibit receptor and non-receptor tyrosine kinases as an approach towards developing new therapeutic agents (see,

25 e.g., Levitzki and Gazit, 1995).

> The structure coordinates described herein can be used as phasing models for determining the crystal structures of additional native or mutated tyrosine kinase domains, as well as the structures of co-crystals of such domains with ligands such as inhibitors, agonists, antagonists, and other molecules. The

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structure coordinates, as well as models of the three-dimensional structures obtained therefrom, can also be used to aid the elucidation of solution-based structures of native or mutated tyrosine kinase domains, such as those obtained via NMR. Thus, the crystals and atomic structure coordinates of the invention provide a convenient means for elucidating the structures and functions of receptor and non-receptor tyrosine kinases.

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For purposes of clarity and discussion, the crystals of the invention will be described by reference to specific FGFR1 exemplary crystals. Those skilled in the art will appreciate that the principles described herein are generally applicable to crystals of the tyrosine kinase domain of any cytoplasmic tyrosine kinase that undergoes ligand-induced dimerization or receptor tyrosine kinase, including but not limited to the tyrosine kinases of FIG. 6.

VII. Structure Determination for PTKs with Unknown Structure Using Structural Coordinates

Structural coordinates, such as those set forth in Table 1, Table 2, Table 3, and Table 4, can be used to determine the three dimensional structures of PTKs with unknown structure. The methods described below can apply structural coordinates of a polypeptide with known structure to another data set, such as an amino acid sequence, X-ray crystallographic diffraction data, or nuclear magnetic resonance (NMR) data. Preferred embodiments of the invention relate to determining the three dimensional structures of PTKs and related polypeptides. These include receptor PTKs such as FGF-

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R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK. Non-receptor PTKs such as SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK can also be used in the methods described herein.

Structures Using Amino Acid Homology

Homology modeling is a method of applying structural coordinates of a polypeptide of known structure to the amino acid sequence of a polypeptide of unknown structure. This method is accomplished using a computer representation of the three dimensional structure of a polypeptide or polypeptide complex, the computer representation of amino acid sequences of the polypeptides with known and unknown structures, and standard computer representations of the structures of amino acids. Homology modeling comprises the steps of (a) aligning the amino acid sequences of the polypeptides with and without known structure; (b) transferring the coordinates of the conserved amino acids in the known structure to the corresponding amino acids of the polypeptide of unknown structure; refining the subsequent three dimensional structure; and (d) constructing structures of the rest of the polypeptide. One skilled in the art recognizes that conserved amino acids between two proteins can be determined from the sequence alignment step in step (a).

The above method is well known to those skilled in the art. Greer, 1985, Science 228, 1055. Blundell et al., 1988, Eur. J. Biochem. 172, 513. A computer program currently utilized for homology modeling by

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those skilled in the art is the Homology module in the Insight II modeling package distributed by Molecular Simulations Inc.

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Alignment of the amino acid sequence is accomplished by first placing the computer representation of the amino acid sequence of a polypeptide with known structure above the amino acid sequence of the polypeptide of unknown structure. Amino acids in the sequences are then compared and groups of amino acids that are homologous (e.g., amino acid side chains that are similar in chemical nature - aliphatic, aromatic, polar, or charged) are grouped together. This method will detect conserved regions of the polypeptides and account for amino acid insertions or deletions.

Once the amino acid sequences of the polypeptides with known and unknown structures are aligned, the structures of the conserved amino acids in the computer representation of the polypeptide with known structure are transferred to the corresponding amino acids of the polypeptide whose structure is unknown. For example, a tyrosine in the amino acid sequence of known structure may be replaced by a phenylalanine, the corresponding homologous amino acid in the amino acid sequence of unknown structure.

The structures of amino acids located in non-conserved regions are to be assigned manually by either using standard peptide geometries or molecular simulation techniques, such as molecular dynamics. The final step in the process is accomplished by refining the entire structure using molecular dynamics and/or energy minimization.

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The homology modeling method is well known to those skilled in the art and has been practiced using different protein molecules. The three dimensional structure of the polypeptide corresponding to the catalytic domain of a serine/threonine protein kinase, myosin light chain protein kinase, was homology modeled from the cAMP-dependent protein kinase catalytic subunit. Knighton et al., 1992, Science 258:130-135.

10 Structures Using Molecular Replacement

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Molecular replacement is a method of applying the X-ray diffraction data of a polypeptide of known structure to the X-ray diffraction data of a polypeptide of unknown sequence. This method can be utilized to define the phases describing the X-ray diffraction data of a polypeptide of unknown structure when only the amplitudes are known. X-PLOR is a commonly utilized computer software package used for molecular replacement. Brünger, 1992, Nature 355:472-475. AMORE is another program used for molecular replacement.

Navaza, 1994, Acta Crystallogr. A50:157-163.

Preferably, the resulting structure does not exhibit a root-mean-square deviation of more than 3 Å.

A goal of molecular replacement is to align the positions of atoms in the unit cell by matching electron diffraction data from two crystals. A program such as X-PLOR can involve four steps. A first step can be to determine the number of molecules in the unit cell and define the angles between them. A second step can involve rotating the diffraction data to define the orientation of the molecules in the unit cell. A third

step can be to translate the electron density in three dimensions to correctly position the molecules in the unit cell. Once the amplitudes and phases of the X-ray diffraction data is determined, an R-factor can be calculated by comparing electron diffraction maps calculated experimentally from the reference data set and calculated from the new data set. An R-factor between 30-50% indicates that the orientations of the atoms in the unit cell are reasonably determined by this method. A fourth step in the process can be to decrease the R-factor to roughly 20% by refining the new electron density map using iterative refinement techniques described herein and known to those or ordinary skill in the art.

Structures Using NMR Data

Structural coordinates of a polypeptide or polypeptide complex derived from X-ray crystallographic techniques can be applied towards the elucidation of three dimensional structures of polypeptides from nuclear magnetic resonance (NMR) data. This method is used by those skilled in the art. Wuthrich, 1986, John Wiley and Sons, New York:176-199; Pflugrath et al., 1986, J. Molecular Biology 189:383-386; Kline et al., 1986, J. Molecular Biology 189:377-382. While the secondary structure of a polypeptide is often readily determined by utilizing two-dimensional NMR data, the spatial connections between individual pieces of secondary structure are not as readily determinable. The coordinates defining a three-dimensional structure of a polypeptide derived from X-ray crystallographic

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techniques can guide the NMR spectroscopist to an understanding of these spatial interactions between secondary structural elements in a polypeptide of related structure.

The knowledge of spatial interactions between secondary structural elements can greatly simplify

Nuclear Overhauser Effect (NOE) data from twodimensional NMR experiments. Additionally, applying the crystallographic coordinates after the determination of secondary structure by NMR techniques only simplifies the assignment of NOEs relating to particular amino acids in the polypeptide sequence and does not greatly bias the NMR analysis of polypeptide structure.

Conversely, using the crystallographic coordinates to simplify NOE data while determining secondary structure of the polypeptide would bias the NMR analysis of protein structure.

As the analysis of polypeptide structure by NMR methods is a relatively new technique, the use of structural coordinates defining a PTK structure will most likely be utilized more frequently in the near future. As the method progresses, the three dimensional structure analysis of polypeptides of the same size as a PTK catalytic domain will become more frequent.

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VIII. Structure-Based Design of Modulators of PTK
Function Utilizing Structural Coordinates
Structure-based modulator design and identification
methods are powerful techniques that can involve
searches of computer data bases containing a wide
variety of potential modulators and chemical functional

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groups. The computerized design and identification of modulators is useful as the computer data bases contain more compounds than the chemical libraries, often by an order of magnitude. For reviews of structure-based drug design and identification see Kuntz et al., 1994, Acc. Chem. Res. 27:117; Guida, 1994, Current Opinion in Struc. Biol. 4: 777; Colman, 1994, Current Opinion in Struc. Biol. 4: 868.

The three dimensional structure of a polypeptide defined by structural coordinates can be utilized by these design methods. The structural coordinates of Table 1, Table 2, Table 3, and Table 4 can be utilized by this method. In addition, the three dimensional structures of receptor and non-receptor PTKs determined by the homology, molecular replacement, and NMR techniques described herein can also be applied to modulator design and identification methods. Thus, the structures of receptor PTKs, FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK, can be utilized by the methods described herein. The structures of non-receptor PTKs, SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK, can also be utilized by the rational modulator design method.

25 <u>Design by Searching Molecular Data Bases</u>

One method of rational modulator design searches for modulators by docking the computer representation of compounds from a data base of molecules. Publicly available data bases include:

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a) ACD from Molecular Designs Limited

- b) NCI from National Cancer Institute
- c) CCDC from Cambridge Crystallographic Data Center
- d) CAST from Chemical Abstract Service
- e) Derwent from Derwent Information Limited
- 5 f) Maybridge from Maybridge Chemical Company LTD
 - g) Aldrich from Aldrich Chemical Company
 - h) Directory of Natural Products from Chapman & Hall

One such data base (ACD distributed by Molecular Designs

Limited Information Systems) contains, for example,

200,000 compounds that are synthetically derived or are
natural products. Methods available to those skilled in
the art can convert a data set represented in two
dimensions to one represented in three dimensions.

These methods are enabled by such computer programs as CONCORD from Tripos Associates or DB-Converter from Molecular Simulations Limited.

Multiple methods of structure-based modulator design are known to those in the art. Kuntz et al., 1982, J. Mol. Biol. 162: 269; Kuntz et al., 1994, Acc. Chem. Res. 27: 117; Meng et al., 1992, J. Compt. Chem. 13: 505; Bohm, 1994, J. Comp. Aided Molec. Design 8: 623.

A computer program widely utilized by those skilled
in the art of rational modulator design is DOCK from the
University of California in San Francisco. The general
methods utilized by this computer program and programs
like it are described in three applications below. More
detailed information regarding some of these techniques
can be found in the Molecular Simulations User Guide,
1995.

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A typical computer program used for this purpose can comprise the following steps:

- (a) remove the existing compound from the protein;
- (b) dock the structure of another compound into the active-site using the computer program (such as DOCK) or by interactively moving the compound into the active-site;
- (c) characterize the space between the compound and the active-site atoms;
- (d) search libraries for molecular fragments which (i)can fit into the empty space between the compound and the active-site, and (ii) can be linked to the compound; and
 - (e) link the fragments found above to the compound and evaluate the new modified compound.

Part (c) refers to characterizing the geometry and the complementary interactions formed between the atoms of the active-site and the compounds. A favorable geometric fit is attained when a significant surface area is shared between the compound and active-site atoms without forming unfavorable steric interactions.

One skilled in the art would note that the method can be performed by skipping parts (d) and (e) and screening a data base of many compounds.

Structure-based design and identification of modulators of PTK function can be used in conjunction with assay screening. As large computer data base of compounds (around 10,000 compounds) can be searched in a matter of hours, the computer based method can narrow the compounds tested as potential modulators of PTK function in cellular assays.

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The above descriptions of structure-based modulator design are not all encompassing and other methods are reported in the literature:

- (1) CAVEAT: Bartlett et al.,1989, in "Chemical and Biological Problems in Molecular Recognition", Roberts, S.M.; Ley, S.V.; Campbell, M.M. eds.; Royal Society of Chemistry: Cambridge, pp182-196.
 - (2) FLOG: Miller et al., 1994, J. Comp. Aided Molec. Design 8:153.
- 10 (3) PRO Modulator: Clark et al., 1995, J. Comp. Aided Molec. Design 9:13.
 - (4) MCSS: Miranker and Karplus, 1991, Proteins: Structure, Function, and Genetics 11:29.
- (5) AUTODOCK: Goodsell and Olson, 1990, Proteins:15 Structure, Function, and Genetics 8:195.
 - (6) GRID: Goodford, 1985, J. Med. Chem. 28:849.

Design by Modifying Compounds in Complex with PTKs
Another way of identifying compounds as potential
modulators is to modify an existing modulator in the
polypeptide active-site. For example, the computer
representation of modulators can be modified within the
computer representation of a PTK active-site. Detailed
instructions for this technique can be found in the
Molecular Simulations User Manual, 1995 in LUDI. The
computer representation of the modulator is modified by
the deletion of a chemical group or groups or by the
addition of a chemical group or groups.

Upon each modification to the compound, the atoms of the modified compound and active-site can be shifted in conformation and the distance between the modulator

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and the active-site atoms may be scored along with any complimentary interactions formed between the two molecules. Scoring can be complete when a favorable geometric fit and favorable complementary interactions are attained. Compounds that have favorable scores are potential modulators of PTK function.

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Design by Modifying the Structure of Compounds that Bind PTKs

10 A third method of structure-based modulator design is to screen compounds designed by a modulator building or modulator searching computer program. Examples of these types of programs can be found in the Molecular Simulations Package, Catalyst. Descriptions for using this program are documented in the Molecular Simulations User Guide (1995). Other computer programs used in this application are ISIS/HOST, ISIS/BASE, ISIS/DRAW) from Molecular Designs Limited and UNITY from Tripos Associates.

These programs can be operated on the structure of a compound that has been removed from the active-site of the three dimensional structure of a compound-PTK complex. Operating the program on such a compound is preferable since it is in a biologically active conformation.

A modulator construction computer program is a computer program that may be used to replace computer representations of chemical groups in a compound complexed with a PTK with groups from a computer data base. A modulator searching computer program is a computer program that may be used to search computer

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representations of compounds from a computer data base that have similar three dimensional structures and similar chemical groups as compound bound to a PTK.

A typical program can operate by using the following general steps:

- (a) map the compounds by chemical features such as by hydrogen bond donors or acceptors, hydrophobic/lipophilic sites, positively ionizable sites, or negatively ionizable sites;
- (b) add geometric constraints to the mapped features; and
 - (c) search data bases with the model generated in (b).

indolinones, the important chemical features include, but are not limited to, a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Those skilled in the art also recognize that not all of the possible chemical features of the compound need be present in the model of (b). One can use any subset of the model to generate different models for data base searches.

IX. Organic Synthetic Techniques

The versatility of computer-based modulator design and identification lies in the diversity of structures screened by the computer programs. The computer programs can search data bases that contain 200,000 molecules and can modify modulators already complexed with the enzyme with a wide variety of chemical

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functional groups. A consequence of this chemical diversity is that a potential modulator of PTK function may take a chemical form that is not predictable. A wide array of organic synthetic techniques exist in the 5 art to meet the challenge of constructing these potential modulators of PTK function. Many of these organic synthetic methods are described in detail in standard reference sources utilized by those skilled in the art. One example of such a reference is March, 1994, Advanced Organic Chemistry: Reactions, Mechanisms, 10 and Structure, New York, McGraw Hill. Thus, the techniques required to synthesize a potential modulator of PTK function identified by computer-based methods are readily available to those skilled in the art of organic 15 chemical synthesis.

X. <u>Cellular Assays Measuring the Effect of a PTK</u> <u>Modulator in Signal Transduction Pathways</u>

20 Cellular assays can be used to test the activity of a potential modulator of PTK function as well as diagnose a disease associated with inappropriate PTK activity. A potential modulator of PTK function can be tested for activity in vitro by assays that measure the 25 effect of a potential modulator on the autophosphorylation of a particular PTK over-expressed in a cell line. Thus, a modulator that acts as a potent inhibitor of the catalytic domain corresponding to a PTK would decrease the amount of autophosphorylation 30 catalyzed by that PTK. Potential modulators could also be tested for activity in cell growth assays in vitro as well as in animal model assays in vivo.

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In vivo assays are also useful for testing the bioactivity of a potential modulator designed by the methods of the invention.

Materials, methods, and experimental data for these assays are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

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XI. Administration of Modulators of PTK Function as Therapeutics for Disease

Methods of administering compounds to organisms as therapeutics for disease are fully described in WO 96/40116 published on December 19, 1996, entitled "Indolinone Compounds for the Treatment of Disease". This application is incorporated herein by reference in its entirety, including all drawings, figures, and tables.

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EXAMPLES

The examples below are non-limiting and are merely representative of various aspects and features of the present invention. The examples provide illustrative methods for obtaining crystalline forms of protein kinase polypeptides, methods for determining three dimensional structures of these protein kinase polypeptides, and methods for identifying modulators of protein kinases using the three dimensional structures of the protein kinases.

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EXAMPLE 1: X-ray Crystallographic Structure Determination of FGFR1

Polypeptide Synthesis and Isolation

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A recombinant baculovirus was engineered to encode residues 456-765 of human FGFR1. A cleavable N-terminal histidine tag was incorporated to aid in protein purification. Three amino acid substitutions were introduced: Cys-488 to Ala, Cys-584 to Ser and Leu-457 to Val. The two cysteine substitutions were made to prevent the formation of disulfide-linked oligomers, which occurs for the native protein. The substitution Leu-457 to Val introduced a Ncol cloning site near Met-456. The codon for Tyr-766 (TAC) was changed to a stop codon (TAG) and a HindIII-cloning site was generated following this stop codon. These substitutions were introduced into the full length human cDNA of FGFR1 in m13MPI9 by site-directed mutagenesis according to the manufacturer's protocol (Amersham).

HindIII and was ligated into appropriately digested pBlueBac HistagB (Invitrogen). Transfection of insect cells (Sf9) was performed with the BaculoGold transfection system according to the manufacturer's protocol (Pharmingen). Following identification of positive plaques, the recombinant baculovirus was amplified to high titer (5x10' virus particles/ml). Sf9 cells were grown in 175-cm² flasks to a density of 2-3x10' per flask and infected with recombinant baculovirus with a multiplicity of infection (MOI) of 10.

After 48 hr, cells were harvested by centrifugation

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at 3,000g for 35 min at 4°C and then lysed in 25 mM

HEPES (pH 7.5), 150 mM NaCl, 10% glycerol, 1.5 mM MgCl₂

1 % Triton X-100, 10 µg/ml aprotonin, 10 µg/ml

leupeptin, and 1 mM phenylmethylsulfonyl fluoride

(PMSF). Lysates were centrifuged in a Sorval RC 5C

(Dupont) for 1 hr at 4°C at 40,000g followed by

ultracentrifugation in an XL-80 (Beckman) at 100,000g

for 1 hr. After centrifugation, the clarified lysate

was passed over a Ni^{2*} -chelating column (Pharmacia), and
the bound histidine-tagged fusion protein was eluted

with 100 mM imidazole (pH 7.5). Pooled fractions were
loaded onto a Mono Q anion exchange column (Pharmacia)
and eluted with a NaCl gradient from 0 to 500 mM.

The fractions containing the fusion protein were concentrated in a Centricon-30 (Amicon), and the histidine tag was removed by overnight digestion with enterokinase (Biozyme) at 20°C. The digestion was terminated by the addition of aprotonin, leupeptin, PMSF, TPCK, and bovine pancreatic trypsin inhibitor (BPTI). The cleaved kinase domain was then separated from the histidine tag on a Superose 12 size-exclusion column (Pharmacia). The eluted kinase domain was further purified on a Mono Q column. The purified kinase domain was analyzed by N-terminal sequencing and mass spectrometry. Five amino acids (SAAGT) remained from the histidine tag. The predicted molecular mass was confirmed by mass spectrometry.

Crystal Growth

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Purified FGFR1 was concentrated to 20-50 mg/ml and exchanged into 10 mM Tris-HCl (pH 8.0), 10 mM NaCl, and

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2 mM DTT using a Centricon-30. Crystals were grown at 4°C by vapor diffusion in hanging drops containing 2.0 μ l of 10 mg/ml protein solution and 2.0 μ l of reservoir solution: 16% polyethylene glycol (PEG) 10000, 0.3 M (NH,),SO,, 5% ethylene glycol, and 100 mM bis-Tris (pH 6.5).

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Crystals of native FGFR1 were soaked in 500 ml stabilizing solution [25% PEG 10000, 0.3 M (NH4)₂SO₄, 0.1 M Bis-Tris (pH 6.5), 5% ethylene glycol] containing 3
[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2indolinone (1-5 mM) or 3-[4-(4-formylpiperazine-1-yl)benzylidenyl]-2-indolinone (1 mM) at 4°C for 24 to 48
hours. The final soaking concentration of DMSO was
between 1 to 5%. The crystals cracked at higher
concentrations of DMSO.

Co-crystals of FGFR1 with the inhibitors could also be obtained by vapor diffusion in hanging drops containing 2.0 μ l of 10 mg/ml protein solution and 2.0 μ l of reservoir solution containing 1 mM 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone and 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone.

Co-crystals of FGFR1 complexed with AMP-PCP were obtained as described for the creation of native crystals, except that the protein solution additionally contained 10 mM AMP-PCP and 20 mM MgCl₂.

Preparation Of Heavy Atom Derivative Crystals

Heavy atom derivative crystals were obtained by soaking FGFR1 native crystals (C2-A form) in a solution containing ethylmercurithiosalicylic acid (thimerosal),

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KAu(CN)₂ or 4-chloromercuribenzoic acid, as provided in Table 1, infra,, and containing 25% PEG 10000, 0.3M (NH₄)₂SO₄, 5% ethylene glycol or glycerol, and 100 mM bis-Tris (pH 6.5), and were flash-cooled either in liquid nitrogen directly (Synchrotron) or in a dry nitrogen stream at -175°C (rotating anode).

Data Collection and Structure Determination

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For native crystals and crystals comprising the nucleotide analog AMP-PCP, data were collected either on a Rigaku RU-200 rotating anode operated at 50 kV and 100 mA (Cu Kα) and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector, or at beamline X-4A at the National Synchrotron Light Source, Brookhaven National Laboratory. Synchrotron data ($\lambda=1.07\text{\AA}$) were collected on Fuji image plates and read with a Fuji scanner. One cryo-cooled crystal was used for each of the data sets. To obtain cryo-cooled crystals, crystals were soaked in a cryo-protectant solution containing 25% PEG 10000, 0.3 M (NH₄)₂SO₄, 5% ethylene glycol or glycerol and 100 mM bis-Tris (pH 6.5), and were flashcooled either in liquid nitrogen directly (synchrotron data) or in a dry nitrogen stream at -175°C (rotating anode data). All data were processed using DENZO and SCALEPACK. Otwinowski, 1993, "Oscillation data reduction program," Proceedings of the CCP4 Study Weekend, Sawyer et al., eds. (Daresbury, United Kingdom: SERC Daresbury Laboratory), 56-62.

For native crystals and crystals comprising the nucleotide analog AMP-PCP, a molecular replacement solution was found initially for the C2-B crystal form

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using an IRK search model that consisted of polyalanine with the common side chains for residues 993-1263 (FGFR1 residues 475-754), excluding residues 1094-1105 (kinase insert) and 1153-1170 (activation loop). With AMORE (Navaza, 1994, AmoRe: an automated package for molecular replacement," Acta Crystallogr. A50: 157-163), using 80% of the structure factor amplitudes between 15.0 and 3.5 A, one of the two molecules in the asymmetric unit was located. The correlation coefficient (c.c.) for the correct 1-molecule solution was 0.23 (versus 0.20 for the highest incorrect solution). This molecule was rigid body-refined in X-PLOR (Brünger, 1992, X-PLOR (Version 3.1) Manual (New Haven, Conneticut: The Howeard Hughes Medical Institute and Department of Molecular Biophysics and Biochemistry, Yale Uiversity)), first as one rigid body unit, then as two units each comprising a lobe of the kinase. Rigid body refinement (12.0-3.5 Å, F>30) resulted in a relative rotation of the two lobes of ~10° and an increase of the c.c. from 0.20 to 0.25. The rigid body-refined molecule was then used as a new search model in AMORE, and this time both molecules in the asymmetric unit were located. The c.c. for the correct 2-molecule solution was 0.35 (versus 0.27 for the highest incorrect solution).

Multiple cycles of model building and refinement against 6.0-2.4 Å data resulted in the addition to the model of many of the side chains and some of the missing polypeptide chain. Model building was performed using TOM/FRODO (Jones, 1985, "Diffraction methods for biological macromolecules. Interactive computer graphics: FRODO," Methods in Enzymology 115: 157-171)

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and conjugate-gradient minimization and simulated annealing were performed using X-PLOR. Brunger, supra. At this stage, the R-value was 30% (free R-value of 36%). To help expedite model building and refinement, experimental phases were obtained. Because crystals grown in the presence of ethylene glycol were easier to manipulate than those grown in glycerol, several heavy-atom derivative data sets were collected from C2-A crystals that had been soaked in various heavy atom solutions. The C2-B structure was subsequently refined against 6.0-2.4 Å data to an R-value of 23.8% (free R-value of 30.4%) with r.m.s.d. values of 0.008 Å for bond distances and 1.4° for bond angles.

Molecular replacement was used to locate the two FGFR1 molecules (designated FLGK-A and FLGK-B) in the asymmetric unit of the C2-A crystal form. Using AMORE with 80% of structure factor amplitudes between 15.0 and 3.5 Å and the C2-B model, the c.c. for the correct 2molecule solution was 0.62 (versus 0.35 for the highest incorrect solution). Heavy atom positions were determined from difference Fourier maps using the calculated phases from the partial model. Refinement of heavy atom parameters and phase determination were performed with MLPHARE (Otwinowski, 1991, "Maximum likelihood refinement of heavy atom parameters," Isomorphous replacement and anomolous Ssattering, Evans and Leslie eds. (Darsbury, United Kingdom: SERC Daresbury Laboratory), 56-62)). An initial molecular isomorphous replacement (MIR)-phased electron density map was calculated with data between 2.0. and 2.8 Å resolution. This map was improved by solvent

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flattening, histogram matching, and non-crystallographic symmetry (NCS) averaging using DM (Cowtan, 1994, "Protein Crystallography," CCP4 and ESF-EACBM Newsletter (joint) 31: 34-38).

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Refinement of the C2-A FGFR1 structure against 6.0-2.0 Å data proceeded by conjugate-gradient minimization and simulated annealing using X-PLOR. Tight NCS restraints were imposed until data to 2.0 Å resolution were included in the refinement, at which point the restraints were lifted. An overall anisotropic B-value was calculated using X-PLOR and applied to the observed structure factors, reducing the R-value by ~3%. Water molecules whose B-values refined to ≥70 Å² were omitted from the subsequent refinement round. The average Bvalue is 37.5 $Å^2$ for all protein atoms, 35.4 $Å^2$ for protein atoms in FLGK-A, 39.7 Å² for protein atoms in FLGK-B, and 40.2 $Å^2$ for water molecules. The side chains for Cys-603 in FLGK-A and FLGK-B and for Met-534 in FLGK-B have been modeled in two different conformations. Residues that are not included in the atomic model due to poor supporting electron density are for FLGK-A: 456-463, 486-490, 501-504, 580-591, 763-765; and for FLG-B: 456-460, 501-504, 578-593, 646-651, 657-659, 762-765.

The positions of the two AMP-PCP molecules (one per FGFR1 molecule) were easily identified in $2F_{\text{obs}(\text{co-complex})}$ - $F_{\text{calc}(\text{FGPR})}$ difference Fourier maps. The AMP-PCP molecule bound to FLGK-B is less tightly bound and has been modeled with an occupancy of 0.5.

Table A summarizes the X-ray crystallography data sets of FGFR1 derivative crystals that were used to determine the structures of crystalline FGFR1 and

crystalline FGFR1:AMP-PCP co-complex of the invention.

TABLE 5

Data Collection and MIR Phasing Summary								
	Native	AMP-PCP	Thi-1*	Thi-2*	РСМВ*	KAu(CN)		
X-ray source	X-4 A	RU-200	RU-200	RU-200	RU-200	RU-200		
Resolution limit (Å)	2.0	. 2.3	2.6	2.8	2.8	2.8		
Number of sites			4	7	2	2		
Conc. (mM)/time (h)			0.1/24	0.1/48	0.2/2	5.0/72		
R _{sym} b(%)	4.8(19.7) ^c	4.5(23.3)°	5.5	9.8	6.8	6.8		
Total observations	122569	91324	55456	59488	67988	45303		
Unique reflections	50771	31997	42820 ^d	35538d	18619	18202		
Completeness (%)	97.3(96.3)°	95.5(93.7)°	95.0	96.7	98.0	97.7		
Signal (%1>3 σ)	80.7(50.3)°	79.6(51.7)°	69.8	66.8	84.7	77.6		
R _{iso} e(%)	_	• • •	17.1	31.2	15.4	15.2		
Phasing power ^f			1.8	2.0	1.0	0.9		
R _{cullis} #(%)	_	*****	0.55	0.50	0.81	0.84		
Overall FOM ^b 0.60								

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^{&#}x27;Thi-1, Thi-2; ethylmercurithiosalicylic acid (thimerosal); PCMB: 4-chloromercuribenzoic acid.

 $^{{}^{}b}R_{svm} = 100 \text{ x } \Sigma_{b}\Sigma_{i}|I_{i}(h)-\langle I(h)\rangle|/\Sigma_{b}\Sigma_{i}I_{i}(h)$

^{&#}x27;Value in parentheses is for the highest resolution shell.

^dI(+h) and I(-h) processed as independent reflections. Anomalous scattering contributions were included.

 $[^]eR_{iso} = 100 \text{ x } \Sigma_h ||F_p(h)\pm F_p(h)|-|F_{PH}(h)||/\Sigma_h|F_p(h)|, \text{ where } F_p \text{ and } F_{PH} \text{ are the native and derivative structure factors, respectively.}$

Phasing power: r.m.s. heavy atom structure factor / r.m.s. lack of closure (for acentric reflections from 20.0 to 2.8Å).

³⁰ ${}^gR_{cadles} = 100 \times \Sigma_h ||F_{PH}(h)| - F_{H(calc)}(h)|/\Sigma_h|F_{PH}(h) \pm F_p(h)|$ (for centric reflections from 20.0 to 2.8Å). ${}^hFigure of merit: \int P(\phi) \exp(i\phi) d\phi / \int P(\phi) d(\phi)$, where P is the probability distribution of the phase angle ϕ .

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For crystals comprising FGFR1 and compounds 1 and 2, data were collected on a Rigaku RU-200 rotating anode (Cu Ka) operating at 50 kV and 100 mA and equipped with double-focusing mirrors and an R-AXIS IIC image plate detector. One cryo-cooled crystal was used for each of the data sets. Crystals were soaked in a cryo-protectant [25% PEG 10000, 0.3 M (NH.),SO., 5% ethylene glycol, 100 mM bis-Tris (pH 6.5), and 1 mM: 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone (hereafter referred to as compound 1) or 3-[4-(4-formylpiperazine-1-yl-)benzylidenyl]-2-indolinone (hereafter referred to as compound 2) and flash-cooled in a dry nitrogen stream at -175°C. Data were processed using DENZO and SCALEPACK. Otwinowski, 1993,

Proceedings of the CCP4 Study Weekend (Daresbury, United Kingdom: SERC Daresbury Laboratory) pp 56-62.

A summary of the data collection parameters are included in the following Table 6:

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TABLE 6

	Resolution limit (Å)	Observa- tions (N)	Complete- ness (%)	Redundan- cy	R _{sym} * (%)	Signal (I> \signal)
compound	2.5	93535	97.6 (96.1)	2.7	6.8 (23.0)	11.8
compound 2	2.4	94093	99.1 (97.9)	3.3	6.3 (32.2)	11.4

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compound 1 structure: 550 residues, 252 water molecules, 2 compound 1 molecules (4589 atoms) compound 2 structure: 550 residues, 248 water molecules, 2 compound 2 molecules (4646 atoms)

30 <u>Structure Analyses</u>

Atomic superpositions were performed with TOSS

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(Hendrickson, 1979). Per residue solvent accessible surface calculations were done with X-PLOR. The surface area buried in a dimer interface was calculated with GRASP (Nicholls et al., 1991) using a probe radius of 1.4 Å. The stereochemical quality of the atomic model was monitored using PROCHECK (Laskowski et al., 1993, PROCHECK: a computer program to check the stereochemical quality of protein structures," J. Appl. Cryst. 26: 283-291). As defined in PROCHECK, 93% of the residues in the model have main-chain torsion angles in the most favored Ramachandran regions. There are no residues in disallowed regions, and three residues in generously allowed regions: Arg-622 in FLGK-A and FLGK-B and Arg-554 in FLGK-A. The overall G-factor score is 0.42.

Table 7 summarizes the X-ray crystallography refinement parameters of the structures of crystalline FGFR1 and crystalline FGFR1:AMP-PCP co-complex of the invention. Table 8 summarizes the X-ray crystallography refinement parameters for the FGFR1/compound complexes.

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TABLE 7

	Refinement Parameters FGFR1: 550 residues, 252 water molecules (4589 atoms)								
	FGFR1:AMP-PCP	: 550 residues	, 238 water n	nolecules, 2 A	MP-PCP mo	lecules (4638	atoms)		
	Model	d-spacings	Reflection S	R-value ^a					
		(Å)	(N)	(%)	bonds (Å)	angles (°)	B-values ^b (Ų)		
	FGFR1:	6.0-2.0	42548	21.3 (26.2)°	0.008	1.3	1.6		
	FGFR1:AMP-PCP:	6.0-2.3	26729	20.1 (27.5)°	0.009	1.4	1.7		

*R-value = 100 x Σ_h ||F_{obs}(h)| - |F_{calc}(h)|| / Σ_h |F_{obs}(h)| for reflections with F_{obs}>2 σ .

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TABLE 8

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Model	d-spacings (Å)	Reflec- tions	R- value' (N)	bonds (Å)	angles (°)	B- values ⁽ (Å ²)
compound l	6.0-2.4	42548	19.7 (27.0) ^k	0.008	1.3	1.6
compound 2	6.0-2.5	26729	20.0 (28.0) ^k	0.008	1.4	1.7

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15 'For bonded protein atoms.

Atomic Structural Coordinates

Tables 1 and 2 provide the atomic structural coordinates of unphosphorylated FGFR1 and unphosphorylated FGFR1:AMP-PCP co-complex, respectively. In the Tables, coordinates for both of the FGFR1 molecules of the dimer comprising the asymmetric unit are provided. The amino acid residue numbers coincide with those used in FIG. 3. In the first FGFR1 molecule of the dimer the residue number is preceded by a 1, i.e., residue number 464 of the first FGFR1 molecule of the dimer is denoted by "1464". Tables 3 and 4 provide the atomic structural coordinates of FGFR1 in complex with indolinone compounds found to inhibit FGFR1 function.

^bFor bonded protein atoms.

^{&#}x27;Value in parentheses is the free R-value (Brünger, 1993) determined from 5% of the data.

 $^{{}^{}a}R_{sym} = 100 \times S_{b}S_{i} |I_{i}(h) - I(h)^{0}| / S_{b}S_{i} |I_{i}(h)$

[&]quot;Value in parentheses is for the highest resolution shell.

ⁱR-value = $100 \times S_h ||F_o(h)| - |F_c(h)|| / S_h ||F_o(h)||$, where F_o and F_c are the observed and calculated structure factors, respectively ($F_o > 2s$).

^{*}Value in parentheses is the free R-value determined from 5% of the data.

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The following abbreviations are used in the Tables:

"Atom Type" refers to the element whose coordinates are provided. The first letter in the column defines the element.

5 "A.A." refers to amino acid.

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"X. Y and Z" provide the Cartesian coordinates of the element.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"OCC" refers to occupancy, and represents the percentage of time the atom type occupies the particular coordinate. OCC values range from 0 to 1, with 1 being 100%.

"PRT1" or "PRT2" relate to occupancy, with PRT1 designating the coordinates of the atom when in the first conformation and PRT2 designating the coordinates of the atom when in the second or alternate conformation.

Structural coordinates for FGFR1 may be modified by mathematical manipulation. Such manipulations include, but are not limited to, crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, inversion of the raw structure coordinates and any combination of the above.

In addition, the structural coordinates can be slightly modified and still render nearly identical three dimensional structures. Therefore, a measure of a unique set of structural coordinates is the root-mean-square deviation of the resulting structure. Structural

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coordinates that render three dimensional structures that deviate from one another by a root-mean-square deviation of less than 1.5 Å may be viewed as identical.

5 EXAMPLE 2: Computer-Based Design of Modulators of PTK Function

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Potential modulators of PTK function were designed and identified by operating the program Catalyst on the structure of 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone. The chemical features constraining the search model include a hydrogen bond donor, a hydrogen bond acceptor, and two hydrophobic points of contact. Approximately 40 compounds were identified as potential modulators of PTK function using this method.

The compounds identified by the method as potential modulators of PTK function were commercially available. These compounds were then tested for their ability to inhibit the FLK PTK in an enzyme linked immunosorbant assay (ELISA). The method of performing this assay is taught in WO 96/40116, entitled "Indolinone Compounds for the Treatment of Disease," published on December 19, 1996, invented by Tang et al., incorporated by reference herein in its entirety, including all figures, drawings, and tables. Flk-1 specific antibodies can be prepared from the following protocol:

Prepare a Tresyl-Activated Agarose/Flk-1-D column
 by incubating 10 ml of Tresyl-Activated Agarose
 with 20 mg of purified GST-Flk-1-D fusion protein

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in 100mM sodium bicarbonate (pH 9.6) buffer overnight at 4°C.

- 2. Wash the column once with PBS.
- 3. Block the excess sites on the column with 2 M glycine for 2 hours at 4°C.
- 4. Wash the column with PBS.
- 5. Incubate the column with Rabbit anti-Flk-1D production bleed for 2 hours at 4°C.
- 6. Wash the column with PBS.
- 7. Elute antiserum with 100 mM Citric Acid, pH3.0 and neutralize the eluate immediately with 2 M Tris, pH 9.0.
 - 8. Dialyize the eluate against PBS overnight at 4oC with 3 changes of buffer (sample to buffer ratio is 1:100).
 - 9. Adjust the dialyized antiserum to 5% glycerol and store at -80°C in small aliquotes.

The Flk-1 ELISA can include a 2,2-azino-bis(3-20 ethylbenz-thiazoline-6-sulfonic acid (ABTS) solution, which can comprise 100mM citric acid (anhydrous), 250 mM Na₂HPO₄ (pH 4.0), 0.5 mg/ml ABTS (Sigma catalog no. A-1888). The solution is most appropriately stored in dark at 4°C until ready for use.

The FLK-1 specific antibodies can also be purchased from Santa Cruz Biotechnology (Catalog No. SC-504).

Four of the forty compounds identified as potential modulators of PTK function were potent modulators of FLK function. These molecules have the following

30 structures:

The modulators inhibit the FLK protein kinase with the following IC_{50} values:

TABLE 9

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Compound	FLK kinase IC ₅₀ (μM) compounds tested at 100μM	FLK kinase IC ₅₀ (μΜ) compounds tested at 20μΜ	EGFR IC ₅₀ (μΜ)	IGF-1R 1C _{so} (μM)
l	14.8	14	>100	>100
2	15.7	10.6	>100	>100
3	21.4	16.6	68	30.9
4	22.9	16.4	>100	>100

The invention illustratively described herein may be practiced in the absence of any element or elements, limitation or limitations which is not specifically disclosed herein. The terms and expressions which have

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been employed are used as terms of description and not of limitation, and there is no intention that in the use of such terms and expressions of excluding any equivalents of the features shown and described or portions thereof, but it is recognized that various modifications are possible within the scope of the invention claimed. Thus, it should be understood that although the present invention has been specifically disclosed by preferred embodiments and optional features, modification and variation of the concepts herein disclosed may be resorted to by those skilled in the art, and that such modifications and variations are considered to be within the scope of this invention as

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Those references not previously incorporated herein by reference, including both patent and non-patent references, are expressly incorporated herein by reference for all purposes. Other embodiments are within the following claims.

defined by the appended claims.

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SEQUENCE LISTING

(i) APPLICANT: SUGEN, INCORPORATED

351 Galveston Drive Redwood City, CA 94063

(ii) TITLE OF INVENTION: CRYSTAL STRUCTURES OF A

PROTEIN TYROSINE KINASE

(iii) NUMBER OF SEQUENCES: 5

(iv) CORRESPONDENCE ADDRESS:

(A) ADDRESSEE: Lyon & Lyon

(B) STREET: 633 West Fifth Street

Suite 4700

(C) CITY: Los Angeles

(D) STATE: California

(E) COUNTRY: U.S.A.

(F) ZIP: 90071-2066

(v) COMPUTER READABLE FORM:

(A) MEDIUM TYPE: 3.5" Diskette, 1.44 Mb

storage

(B) COMPUTER: IBM Compatible

(C) OPERATING SYSTEM: IBM P.C. DOS 5.0

(D) SOFTWARE: FastSEQ for Windows 2.0

(vi) CURRENT APPLICATION DATA:

(A) APPLICATION NUMBER: To Be Assigned

(B) FILING DATE: Herewith

(C) CLASSIFICATION:

(vii) PRIOR APPLICATION DATA:

(A) APPLICATION NUMBER:

(B) FILING DATE:

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(viii) ATTORNEY/AGENT INFORMATION:

(A) NAME: Warburg, Richard J.

(B) REGISTRATION NUMBER: 32,327

(C) REFERENCE/DOCKET NUMBER: 227/088-PCT

(ix) TELECOMMUNICATION INFORMATION:

(A) TELEPHONE: (213) 489-1600 (B) TELEFAX: (213) 955-0440

(C) TELEX: 67-3510

(2) INFORMATION FOR SEQ ID NO:1:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 310 amino acids

(B) TYPE: amino acid

(C) STRANDEDNESS: single

(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:1:

Met Leu Ala Gly Val Ser Glu Tyr Glu Leu Pro Glu Asp Pro Arg Trp

1 5 10 15

Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys Pro Leu Gly Glu Gly 20 25 30

Cys Phe Gly Gln Val Val Leu Ala Glu Ala Ile Gly Leu Asp Lys Asp 35 40 45

Lys Pro Asn Arg Val Thr Lys Val Ala Val Lys Met Leu Lys Ser Asp 50 55 60

Ala Thr Glu Lys Asp Leu Ser Asp Leu Ile Ser Glu Met Glu Met 65 70 75 80

Lys Met Ile Gly Lys His Lys Asn Ile Ile Asn Leu Leu Gly Ala Cys
85 90 95

Thr Gln Asp Gly Pro Leu Tyr Val Ile Val Glu Tyr Ala Ser Lys Gly 100 105 110

Asn Leu Arg Glu Tyr Leu Gln Ala Arg Arg Pro Pro Gly Leu Glu Tyr 115 120 125

Cys Tyr Asn Pro Ser His Asn Pro Glu Glu Gln Leu Ser Ser Lys Asp 130 135 140

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Leu Val Ser Cys Ala Tyr Gln Val Ala Arg Gly Met Glu Tyr Leu Ala 145 150 155 160

Ser Lys Lys Cys Ile His Arg Asp Leu Ala Ala Arg Asn Val Leu Val 165 170 175

Thr Glu Asp Asn Val Met Lys Ile Ala Asp Phe Gly Leu Ala Arg Asp 180 185 190

Ile His His Ile Asp Tyr Tyr Lys Lys Thr Thr Asn Gly Arg Leu Pro 195 200 205

Val Lys Trp Met Ala Pro Glu Ala Leu Phe Asp Arg Ile Tyr Thr His 210 215 220

Gln Ser Asp Val Trp Ser Phe Gly Val Leu Leu Trp Glu Ile Phe Thr 225 230 235 240

Leu Gly Gly Ser Pro Tyr Pro Gly Val Pro Val Glu Glu Leu Phe Lys
245 250 255

Leu Leu Lys Glu Gly His Arg Met Asp Lys Pro Ser Asn Cys Thr Asn 260 265 270

Glu Leu Tyr Met Met Met Arg Asp Cys Trp His Ala Val Pro Ser Gln 275 280 285

Arg Pro Thr Phe Lys Gln Leu Val Glu Asp Leu Asp Arg Ile Val Ala 290 295 300

Leu Thr Ser Asn Gln Glu 305 310

(2) INFORMATION FOR SEQ ID NO:2:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 315 amino acids

(B) TYPE: amino acid (C) STRANDEDNESS: single

(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:2:

Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu Tyr Glu Leu Pro 1 5 10 15

Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu Val Leu Gly Lys
20 25 30

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Pro	Leu	Gly 35	Glu	Gly	Ala	Phe	Gly 40	Gln	Val	Val	Leu	Ala 45	Glu	Ala	Ile
Gly	Leu 50	Asp	Lys	Asp	Lys	Pro 55	Asn	Arg	Val	Thr	Lys 60	Val	Ala	Val	Lys
Met 65	Leu	Lys	Ser	Asp	Ala 70	Thr	Glu	Lys	Asp	Leu 75	Ser	Asp	Leu	Ile	Ser 80
Glu	Met	Glu	Met	Met 85	Lys	Met	Ile	Gly	Lys 90	His	Lys	Asn	Ile	Ile 95	Asn
Leu	Leu	Gly	Ala 100	Cys	Thr	Gln	Asp	Gly 105	Pro	Leu	Tyr	Val	Ile 110	Val	Glu
Tyr	Ala	Ser 115	Lys	Gly	Asn	Leu	Arg 120	Glu	Tyr	Leu	Gln	Ala 125	Arg	Arg	Pro
Pro	Gly 130	Leu	Glu	Tyr	Ser	Tyr 135	Asn	Pro	Ser	His	Asn 140	Pro	Glu	Glu	Gln
Leu 145	Ser	Ser	Lys	Asp	Leu 150	Val	Ser	Cys	Ala	Tyr 155	Gln	Val	Ala	Arg	Gly 160
Met	Glu	Tyr	Leu	Ala 165	Ser	Lys	Lys	Суѕ	Ile 170	His	Arg	Asp	Leu	Ala 175	Ala
Arg	Asn	Val	Leu 180	Val	Thr	Glu	Asp	Asn 185	Val	Met	Lys	Ile	Ala 190	Ąsp	Phe
Gly	Leu	Ala 195	Arg	Asp	Ile	His	His 200	Ile	Asp	Tyr	Tyr	Lys 205	Lys	Thr	Thr
Asn	Gly 210	Arg	Leu	Pro	Val	Lys 215	Trp	Met	Ala	Pro	Glu 220	Ala	Leu	Phe	Asp
Arg 225	Ile	Tyr	Thr	His	Gln 230	Ser	Asp	Val	Trp	Ser 235	Phe	Gly	Val	Leu	Leu 240
Trp	Glu	Ile	Phe	Thr 245	Leu	Gly	Gly	Ser	Pro 250	Tyr	Pro	Gly	Val	Pro 255	Val
Glu	Glu	Leu	Phe 260	Lys	Leu	Leu	Lys	Glu 265	Gly	His	Arg	Met	Asp 270	Lys	Pro
Ser	Asn	Cys 275	Thr	Asn	Glu	Leu	Tyr 280	Met	Met	Met	Arg	Asp 285	Cys	Trp	His
Ala	Val 290	Pro	Ser	Gln	Arg	Pro 295	Thr	Phe	Lys	Gln	Leu 300	Val	Glu	Asp	Leu
Asp 305	Arg	Ile	Val	Ala	Leu 310	Thr	Ser	Asn	Gln	Glu 315					

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(2) INFORMATION FOR SEQ ID NO:3:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 351 amino acids

(B) TYPE: amino acid

(C) STRANDEDNESS: single
(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: protein

(iii) HYPOTHETICAL: NO

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:3:

Met Arg Gly Ser His His His His His Gly Met Ala Ser Met Thr
1 5 10 15

Gly Gly Gln Met Gly Arg Asp Leu Tyr Asp Asp Asp Asp Lys Asp 20 25 30

Pro Ser Ser Arg Ser Ala Ala Gly Thr Met Val Ala Gly Val Ser Glu 35 40 45

Tyr Glu Leu Pro Glu Asp Pro Arg Trp Glu Leu Pro Arg Asp Arg Leu 50 55 60

Val Leu Gly Lys Pro Leu Gly Glu Gly Ala Phe Gly Gln Val Val Leu 65 70 75 80

Ala Glu Ala Ile Gly Leu Asp Lys Asp Lys Pro Asn Arg Val Thr Lys
85 90 95

Val Ala Val Lys Met Leu Lys Ser Asp Ala Thr Glu Lys Asp Leu Ser 100 105 110

Asp Leu Ile Ser Glu Met Glu Met Met Lys Met Ile Gly Lys His Lys 115 120 125

Asn Ile Ile Asn Leu Leu Gly Ala Cys Thr Gln Asp Gly Pro Leu Tyr 130 135 140

Val Ile Val Glu Tyr Ala Ser Lys Gly Asn Leu Arg Glu Tyr Leu Gln 145 150 155 160

Ala Arg Arg Pro Pro Gly Leu Glu Tyr Ser Tyr Asn Pro Ser His Asn 165 170 175

Pro Glu Glu Gln Leu Ser Ser Lys Asp Leu Val Ser Cys Ala Tyr Gln 180 185 190

Val Ala Arg Gly Met Glu Tyr Leu Ala Ser Lys Lys Cys Ile His Arg 195 200 205

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Asp	Leu 210	Ala	Ala	Arg	Asn	Val 215	Leu	Val	Thr	Glu	Asp 220	Asn	Val	Met	Lys
Ile 225	Ala	Asp	Phe	Gly	Leu 230	Ala	Arg	Asp	Ile	His 235	His	Ile	Asp	Tyr	Tyr 240
Lys	Lys	Thr	Thr	Asn 245	Gly	Arg	Leu	Pro	Val 250	Lys	Trp	Met	Ala	Pro 255	Glu
Ala	Leu	Phe	Asp 260	Arg	Ile	Tyr	Thr	His 265	Gln	Ser	Asp	Val	Trp 270	Ser	Phe
Gly	Val	Leu 275	Leu	Trp	Glu	Ile	Phe 280	Thr	Leu	Gly	Gly	Ser 285	Pro	Tyr	Pro
Gly	Val 290	Pro	Val	Glu	Glu	Leu 295	Phe	Lys	Leu	Leu	Lys 300	Glu	Gly	His	Arg
Met 305	Asp	Lys	Pro	Ser	Asn 310	Суз	Thr	Asn	Glu	Leu 315	Tyr	Met	Met	Met	Arg 320
Asp	Cys	Trp	His	Ala 325	Val	Pro	Ser	Gln	Arg 330	Pro	Thr	Phe	Lys	Gln 335	Leu
Val	Glu	Asp	Leu 340	Asp	Arg	Ile	Val	Ala 345	Leu	Thr	Ser	Asn	Gln 350	Glu	

(2) INFORMATION FOR SEQ ID NO:4:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 933 base pairs
(B) TYPE: nucleic acid
(C) STRANDEDNESS: double

(D) TOPOLOGY: linear

(ii) MOLECULE TYPE: cDNA to mRNA

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:4:

ATGCTAGCAG GGGTCTCTGA GTATGAGCTT CCCGAAGACC CTCGCTGGGA GCTGCCTCGG 60
GACAGACTGG TCTTAGGCAA ACCCCTGGGA GAGGGCTGCT TTGGGCAGGT GGTGTTGGCA 120
GAGGCTATCG GGCTGGACAA GGACAAACCC AACCGTGTGA CCAAAGTGGC TGTGAAGATG 180
TTGAAGTCGG ACGCAACAGA GAAAGACTTG TCAGACCTGA TCTCAGAAAT GGAGATGATG 240
AAGATGATCG GGAAGCATAA GAATATCATC AACCTGCTGG GGGCCTGCAC GCAGGATGGT 300
CCCCTTGTATG TCATCGTGGA GTATGCCTCC AAGGGCAACC TGCGGGAGTA CCTGCAGGCC 360
CGGAGGCCCC CAGGGCTGGA ATACTGCTAC AACCCCAGCC ACAACCCAGA GGAGCAGCTC 420

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TCCTCCAAGG	ACCTGGTGTC	CTGCGCCTAC	CAGGTGGCCC	GAGGCATGGA	GTATCTGGCC	480
TCCAAGAAGT	GCATACACCG	AGACCTGGCA	GCCAGGAATG	TCCTGGTGAC	AGAGGACAAT	540
GTGATGAAGA	TAGCAGACTT	TGGCCTCGCA	CGGGACATTC	ACCACATCGA	СТАСТАТААА	600
AAGACAACCA	ACGGCCGACT	GCCTGTGAAG	TGGATGGCAC	CCGAGGCATT	ATTTGACCGG	660
ATCTACACCC	ACCAGAGTGA	TGTGTGGTCT	TTCGGGGTGC	TCCTGTGGGA	GATCTTCACT	720
CTGGGCGGCT	CCCCATACCC	CGGTGTGCCT	GTGGAGGAAC	TTTTCAAGCT	GCTGAAGGAG	780
GGTCACCGCA	TGGACAAGCC	CAGTAACTGC	ACCAACGAGC	TGTACATGAT	GATGCGGGAC	840
TGCTGGCATG	CAGTGCCCTC	ACAGAGACCC	ACCTTCAAGC	AGCTGGTGGA	AGACCTGGAC	900
CGCATCGTGG	CCTTGACCTC	CAACCAGGAG	TAG			933

(2) INFORMATION FOR SEQ ID NO:5:

(i) SEQUENCE CHARACTERISTICS:

(A) LENGTH: 1056 base pairs
(B) TYPE: nucleic acid

(C) STRANDEDNESS: double

(D) TOPOLOGY:

linear

(ii) MOLECULE TYPE:

CDNA

(xi) SEQUENCE DESCRIPTION: SEQ ID NO:5:

ATGCGGGGTT	CTCATCATCA	TCATCATCAT	GGTATGGCTA	GCATGACTGG	TGGACAGCAA	60
ATGGGTCGGG	ATCTGTACGA	CGATGACGAT	AAGGATCCGA	GCTCGAGATC	TGCAGCTGGT	120
ACCATGGTAG	CAGGGGTCTC	TGAGTATGAG	CTTCCCGAAG	ACCCTCGCTG	GGAGCTGCCT	180
CGGGACAGAC	TGGTCTTAGG	CAAACCCCTG	GGAGAGGGCG	CCTTTGGGCA	GGTGGTGTTG	240
GCAGAGGCTA	TCGGGCTGGA	CAAGGACAAA	CCCAACCGTG	TGACCAAAGT	GGCTGTGAAG	300
ATGTTGAAGT	CGGACGCAAC	AGAGAAAGAC	TTGTCAGACC	TGATCTCAGA	AATGGAGATG	360
ATGAAGATGA	TCGGGAAGCA	TAAGAATATC	ATCAACCTGC	TGGGGGCCTG	CACGCAGGAT	420
GGTCCCTTGT	ATGTCATCGT	GGAGTATGCC	TCCAAGGGCA	ACCTGCGGGA	GTACCTGCAG	480
GCCCGGAGGC	CCCCAGGGCT	GGAATACTCC	TACAACCCCA	GCCACAACCC	AGAGGAGCAG	540
CTCTCCTCCA	AGGACCTGGT	GTCCTGCGCC	TACCAGGTGG	CCCGAGGCAT	GGAGTATCTG	600
GCCTCCAAGA	AGTGCATACA	CCGAGACCTG	GCAGCCAGGA	ATGTCCTGGT	GACAGAGGAC	660

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AATGTGATGA	AGATAGCAGA	CTTTGGCCTC	GCACGGGACA	TTCACCACAT	CGACTACTAT	720
AAAAA GACAA	CCAACGGCCG	ACTGCCTGTG	AAGTGGATGG	CACCCGAGGC	ATTATTTGAC	780
CGGATCTACA	CCCACCAGAG	TGATGTGTGG	TCTTTCGGGG	TGCTCCTGTG	GGAGATCTTC	840
ACTCTGGGCG	GCTCCCCATA	CCCCGGTGTG	CCTGTGGAGG	AACTTTTCAA	GCTGCTGAAG	900
GAGGGTCACC	GCATGGACAA	GCCCAGTAAC	TGCACCAACG	AGCTGTACAT	GATGATGCGG	960
GACTGCTGGC	ATGCAGTGCC	CTCACAGAGA	CCCACCTTCA	AGCAGCTGGT	GGAAGACCTG	1020
GACCGCATCG	TGGCCTTGAC	CTCCAACCAG	GAGTAG		•	1056

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TABLE 1

At No	om	Atom Type	A.A	A.A No.	x	Y	Z	occ	В	
ATOM	1	N	GLU	1464	-13.639	16.975	8.571	1.00	54.29	
ATOM	3	CA	GLU	1464	-12.479	17.105	7.695	1.00	52.62	
ATOM	4	CB	GLU	1464	-11.400	17.974	8.349	1.00	54.64	
ATOM	5	C	GLU	1464	-11.914	15.738	7.319	1.00	49.74	
MOTA	6	0	GLU	1464	~11.845	15.407	6.136	1.00	52.04	
ATOM	7	N	LEU	1465	-11.562	14.925	8.310	1.00	44.95	
MOTA	9	CA	LEU	1465	-11.018	13.599	8.037	1.00	41.04	
ATOM	10	СВ	LEU	1465	-10.236	13.066	9.235	1.00	40.18	
ATOM	11	CG	LEU	1465	-8.719	13.196	9.130	1.00	43.70	
ATOM	12	CD1	LEU	1465	-8.346	14.654	8.891	1.00	46.74	
MOTA	13	CD2	LEU	1465	-8.061	12.671	10.395	1.00	40.72	
MOTA	14	С	LEU	1465	-12.092	12.594	7.656	1.00	39.18	
ATOM	15	0	LEU	1465	-13.187	12.590	8.219	1.00	38.05	
ATOM	16	N	PRO	1466	-11.802	11.748	6.657	1.00	37.20	
ATOM ATOM	17	CD	PRO	1466	-10.597	11.793	5.810	1.00	36.41	
ATOM	18	CA	PRO	1466	-12.741	10.727	6.189	1.00	36.13	
	19	CB	PRO	1466	-12.110	10.262	4.878	1.00	37.50	
ATOM ATOM	20 21	CG	PRO	1466	-10.629	10.459	5.135	1.00	36.20	
ATOM	22	С С	PRO	1466	-12.846	9.595	7.201	1.00	35.61	
ATOM	23	Ŋ	PRO GLU	1466	-11.847	9.174	7.788	1.00	35.18	
ATOM	25	CA	GLU	1467	-14.060 -14.268	9.121 8.053	7.429	1.00	35.38	
ATOM	26	CB	GLU	1467			8.377	1.00	35.43	
MOTA	27	CG	GLU	1467 1467	-15.744 -16.375	7.965	8.746	1.00	41.10	
ATOM	28	CD	GLU	1467	-17.819	9.280	9.098	1.00	48.25	
ATOM	29	OE1	GLU	1467	-18.446	9.145 8.071	9.596 9. 378	1.00	50.24	
ATOM	30	OE2	GLU	1467	-18.314	10.109		1.00	52.82	
ATOM	31	C	GLU	1467	-13.838	6.714	10.230 7.801	1.00	51.26	
ATOM	32	o	GLU	1467	-13.899	6.511	6.591	1.00 1.00	32.65 35.06	
ATOM	33	N	ASP	1468	-13.299	5.854	B.659	1.00	30.46	
ATOM	35	CA	ASP	1468	-12.883	4.516	8.262	1.00	28.85	
ATOM	36	СВ	ASP	1468	-11.384	4.424	7.975	1.00	29.34	
ATOM	37	CG	ASP	1468	-10.985	3.072	7.408	1.00	27.57	
MOTA	38	OD1	ASP	1468	-11.833	2.159	7.359	1.00	27.78	
MOTA	39	OD2	ASP	1468	-9.817	2.916	7.003	1.00	30.64	
ATOM	40	С	ASP	1468	-13.252	3.564	9.384	1.00	29.29	
ATOM	41	0	ASP	1468	-12.481	3.364	10.336	1.00	27.76	
ATOM	42	N	PRO	1469	-14.435	2.939	9.268	1.00	28.99	
ATOM	43	CD	PRO	1469	-15.354	3.091	8.120	1.00	28.09	
ATOM	44	CA	PRO	1469	-14.971	1.987	10.244	1.00	30.01	
ATOM	45	CB	PRO	1469	-16.244	1.473	9.553	1.00	33.33	
MOTA	46	CG	PRO	1469	-16.665	2.630	8.690	1.00	30.53	
ATOM	47	С	PRO	1469	-14.012	0.848	10.563	1.00	28.96	
ATOM	48	0	PRO	1469	-14.085	0.251	11.636	1.00	28.52	
ATOM	49	N	ARG	1470	-13.106	0.556	9.631	1.00	27.59	
MOTA	51	CA	ARG	1470	-12.139	-0.520	9.810	1.00	27.37	
ATOM	52	СВ	ARG	1470	-11.301	-0.707	8.533	1.00	28.84	
				_	-				20.03	

ATOM	53	CG	ARG	1470	-12.049	-1.279	7.317	1.00	30.57
ATOM	54	CD	ARG	1470	-11.137	-1.352	6.068	1.00	26.71
ATOM	5 5	NE	ARG	1470	-10.489	-0.068	5.793	1.00	31.26
MOTA	57	CZ	ARG	1470	-9.603	0.151	4.823	1.00	32.60
MOTA	58	NHl	ARG	1470	-9.241	-0.828	3.999	1.00	33.19
MOTA	61	NH2	ARG	1470	-9.067	1.359	4.686	1.00	28.65
ATOM	64	C	ARG	1470	-11.180	-0.285	10.981	1.00	29.21
ATOM	65	0	ARG	1470	-10.757	-1.230	11.641	1.00	28.47
ATOM	66	N	TRP	1471	-10.909	0.977	11.280	1.00	27.80
ATOM	68	CA	TRP	1471	-9.940	1.314	12.306	1.00	28.62
ATOM	69	СВ	TRP	1471	-8.729	1.944	11.609	1.00	24.97
ATOM	70	CG	TRP	1471	-8.044	0.976	10.728	1.00	24.86
ATOM	71	CD2	TRP	1471	-7.156	-0.060	11.144	1.00	
ATOM	72	CE2	TRP	1471	-6.782	-0.776	9.989	1.00	28.00
ATOM	73	CE3	TRP	1471	-6.642				29.23
ATOM	74	CD1	TRP	1471		-0.460	12.389	1.00	26.59
ATOM	75	NE1	TRP	1471	-8.166 -7.413	0.860	9.374	1.00	27.23
ATOM	73 77	CZ2	TRP		-7.413 -5.912	-0.192	8.922	1.00	30.10
ATOM	78	CZ3		1471	-5.912 -5.770	-1.866	10.036	1.00	28.70
ATOM	78 79	CH2	TRP	1471	-5.778	-1.545	12.435	1.00	27.18
ATOM			TRP	1471	~5.424	-2.237	11.266	1.00	27.23
ATOM	80 81	C	TRP	1471	-10.371	2.223	13.440	1.00	28.42
ATOM		0	TRP	1471	-9.664	2.321	14.442	1.00	26.48
MOTA	82	N GD	GLU	1472	-11.521	2.874	13.293	1.00	28.62
	84	CA	GLU	1472	-11.981	3.823	14.297	1.00	27.16
MOTA	85	CB	GLU	1472	-13.245	4.534	13.799	1.00	28.89
MOTA	86	CG	GLU	1472	-13.552	5.869	14.520	1.00	29.09
ATOM	87	CD	GLU	1472	-12.692	7.042	14.054	1.00	26.43
ATOM	88	OE1	GLU	1472	-12.134	7.009	12.938	1.00	28.59
ATOM	89	OE2	GLU	1472	-12.596	8.024	14.801	1.00	27.28
ATOM	90	C	GLU	1472	-12.217	3.269	15.701	1.00	25.10
ATOM	91	0	GLU	1472	-12.763	2.196	15.861	1.00	26.48
ATOM	92	N	LEU	1473	-11.750	3.991	16.711	1.00	24.65
ATOM	94	CA	LEU	1473	-11.962	3.608	18.104	1.00	26.27
ATOM	95	СВ	LEU	1473	-10.645	3.266	18.817	1.00	28.24
ATOM	96	CG	LEU	1473	-10.750	3.025	20.337	1.00	27.23
ATOM	97	CD1	LEU	1473	-11.323	1.636	20.642	1.00	25.23
ATOM	98	CD2	LEU	1473	-9.390	3.183	21.000	1.00	26.33
MOTA	99	С	LEU	1473	-12.546	4.856	18.740	1.00	26.52
MOTA	100	0	LEU	1473	-12.122	5.973	18.411	1.00	25.16
ATOM	101	N	PRO	1474	-13.610	4.703	19.554	1.00	28.52
MOTA	102	CD	PRO	1474	-14.435	3.500	19.770	1.00	29.65
MOTA	103	CA	PRO	1474	-14.215	5.870	20.207	1.00	29.18
MOTA	104	CB	PRO	1474	-15.368	5.251	21.003	1.00	28.58
ATOM	105	CG	PRO	1474	-15.768	4.097	20.154	1.00	28.17
ATOM	106	С	PRO	1474	-13.173	6.528	21.124	1.00	29.75
MOTA	107	0	PRO	1474	-12.427	5.841	21.828	1.00	31.78
ATOM	108	N	ARG	1475	-13.107	7.849	21.097	1.00	30.76
MOTA	110	CA	ARG	1475	-12.149	8.588	21.900	1.00	32.26
MOTA	111	СВ	ARG	1475	-12.362	10.083	21.743	1.00	31.58
MOTA	112	CG	ARG	1475	-12.178	10.536	20.342	1.00	37.54
ATOM	113	CD	ARG	1475	-12.048	12.027	20.206	1.00	36.96
ATOM	114	NE	ARG	1475	-11.733	12.317	18.813	1.00	40.07
ATOM	116	CZ	ARG	1475	-10.503	12.501	18.352	1.00	37.59
MOTA	117	NH1	ARG	1475	-9.470	12.501	19.186	1.00	
	'	7471T	AA.O	T413	3.370	16.34/	17.100	1.00	34.89

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ATOM 120 NH2 **ARG** 1475 -10.308 12.669 17.049 1.00 34.54 **ATOM** 123 C ARG 1475 -12.173 8.261 23.371 1.00 35.58 **ATOM** 124 0 ARG 1475 -11.135 8.318 24.036 1.00 37.03 MOTA 125 N ASP 1476 -13.356 7.958 23.889 1.00 36.68 MOTA 127 CA ASP 1476 -13.498 7.647 25.307 1.00 37.07 ATOM 128 **ASP** CB 1476 -14.967 7.759 25.740 1.00 37.87 MOTA 129 CG **ASP** 1476 -15.851 38.93 6.704 25.115 1.00 MOTA 130 OD1 ASP 1476 -15.412 6.015 24.179 1.00 43.75 **ATOM** 131 OD2 ASP 1476 -17.003 6.558 25.563 1.00 45.77 ATOM 132 С ASP 1476 -12.922 6.292 25.701 1.00 35.86 **ATOM** ASP 133 0 1476 -12.923 5.928 26.878 1.00 37.98 **ATOM** 134 N ARG 1477 -12.478 5.527 24.711 1.00 33.37 **ATOM** 136 CA ARG 1477 -11.889 4.221 24.961 1.00 31:84 MOTA 137 CB ARG 1477 ..-12.214 3.262 23.809 1.00 31.84 ATOM 138 CG ARG 1477 -13.693 2.965 23.580 1.00 29.70 **ATOM** 139 CD ARG 1477 -14.366 2.365 24.809 1.00 33.88 MOTA 140 NE. ARG 1477 -14.596 3.372 25.838 1.00 33.86 MOTA 142 CZ ARG 1477 -14.845 3.102 27.113 1.00 34.14 MOTA 143 NH1 ARG 1477 -14.906 1.846 27.542 1.00 30.58 MOTA 146 NH2 ARG 1477 -15.024 4.102 27.961 1.00 33.14 MOTA 149 C ARG 1477 -10.373 4.338 25.105 1.00 31.30 ATOM 150 0 ARG 1477 -9.679 3.362 25.365 1.00 32.32 ATOM 151 N LEU 1478 -9.856 5.544 24.97B 1.00 32.85 MOTA 153 CA LEU 1478 -8.426 5.739 25.054 1.00 35.64 MOTA 154 CB LEU 34.96 1478 -7.964 6.360 23.737 1.00 MOTA 155 CG LEU 1478 -6.498 6.291 23.331 1.00 36.36 MOTA 156 CD1 LEU 1478 -6.059 4.833 23.192 1.00 30.71 MOTA 157 CD2 LEU 1478 -6.335 7.048 22.020 1.00 33.97 MOTA 158 С LEU 1478 -8.054 6.625 26.243 1.00 37.60 MOTA 159 0 LEU 1478 -8.366 7.815 26.263 1.00 41.20 MOTA 160 N VAL 1479 -7.442 6.023 27.257 1.00 36.52 MOTA 162 CA VAL -7.008 6.745 1479 28.449 1.00 35.59 MOTA 163 CB VAL 1479 -7.041 5.829 29.688 1.00 35.92 MOTA CG1 164 VAL 1479 -6.712 6.627 30.926 1.00 39.40 ATOM 165 CG2 VAL 1479 -8.404 5.163 29.825 1.00 34.46 ATOM-166 C VAL 1479 -5.577 7.224 28.197 1.00 35.36 MOTA 167 0 1479 VAL -4.622 6.443 28.269 1.00 32.50 MOTA 168 N LEU 1480 -5.439 8.506 27.878 1.00 37.77 MOTA 170 CA LEU 1480 -4.132 9.086 27.572 1.00 42.77 MOTA 171 CB LEU 1480 -4.298 10.421 26.842 1.00 41.84 MOTA 172 CG LEU 1480 -4.991 10.369 25.471 1.00 42.45 MOTA 173 CD1 LEU 1480 -5.135 11.774 24.924 1.00 42.58 MOTA 174 CD2 LEU 1480 -4.200 9.508 24.502 1.00 43.09 MOTA 175 C LEU 1480 -3.211 9.233 28.778 1.00 45.25 MOTA 176 O LEU 1480 -3.621 9.739 29.822 1.00 45.47 MOTA 177 N GLY 1481 -1.958 8.816 28.612 1.00 46.82 MOTA 179 CA GLY 1481 -1.016 8.889 29.708 1.00 50.47 MOTA 180 С GLY 1481 0.296 9.617 29.472 1.00 52.24 MOTA 181 O GLY 1481 0.360 10.638 28.781 1.00 53.41 MOTA 182 N LYS 1482 1.349 9.070 30.068 1.00 53.64 MOTA 184 CA LYS 1482 2.697 9.627 30.000 1.00 56.19 MOTA 185 CB LYS 1482 3.636 8.776 30.859 1.00 57.19 ATOM 186 CG LYS 1482 5.115 9.023 30.628 1.00 61.02 MOTA 187 CD LYS 1482 5.938 7.831 31.089 1.00 63.12

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ATOM	188	CE	LYS	1482	5.494	6.547	30.395	1.00	61.98
ATOM	189	NZ	LYS	1482	6.252	5.368	30.899	1.00	63.38
MOTA	193	С	LYS	1482	3.297	9.795	28.604	1.00	56.56
ATOM	194	0	LYS	1482	3.291	8.868	27.791	1.00	55.03
ATOM	195	N	PRO	1483	3.852	10.983	28.323	1.00	58.31
MOTA	196	$^{\text{CD}}$	PRO	1483	3.859	12.191	29.167	1.00	56.98
ATOM	197	CA	PRO	1483	4.465	11.254	27.020	1.00	59.52
ATOM	198	CB	PRO	1483	4.910	12.711	27.155	1.00	58.75
ATOM	199	CG	PRO	1483	3.927	13.278	28.141	1.00	58.79
ATOM	200	С	PRO	1483	5.673	10.335	26.834	1.00	61.17
ATOM	201	0	PRO	1483	6.509	10.216	27.731	1.00	61.31
ATOM	202	N	LEU	1484	5.728	9.643	25.702	1.00	64.31
ATOM	204	CA	LEU	1484	6.838	8.738	25.408	1.00	67.77
ATOM	205	CB	LEU	1484	6.349	7.512		1:00	67.66
MOTA	206	CG	LEU	1484	5.415	6.558	25.386	1.00	69.00
MOTA	207	CD1	LEU	1484	4.943	5.457	24.445	1.00	66.76
ATOM	208	CD2	LEU	1484	6.126	5.972	26.604	1.00	67.77
MOTA	209	С	LEU	1484	7.934	9.431	24.608	1.00	70.82
ATOM	210	0	LEU	1484	9.117	9.115	24.759	1.00	71.82
ATOM	211	N	GLY	1485	7.534	10.357	23.742	1.00	73.28
ATOM	213	CA	GLY	1485	8.492	11.077	22.922	1.00	74.53
MOTA	214	C	GLY	1485	7.819	11.754	21.747	1.00	75.19
MOTA	215	0	GLY	1485	6.635	12.090	21.822	1.00	75.61
MOTA	216	N	GLN	1491	4.406	14.274	18.638	1.00	50.72
MOTA	218	CA	GLN	1491	4.042	13.876	19.994	1.00	47.33
MOTA	219	CB	GLN	1491	3.033	14.869	20.587	1.00	46.67
MOTA	220	C	GLN	1491	3.486	12.449	20.073	1.00	46.66
MOTA	221	0	GLN	1491	2.581	12.074	19.323	1.00	45.20
MOTA	222	N	VAL	1492	4.072	11.650	20.960	1.00	45.41
MOTA	224	CA	VAL	1492	3.646	10.274	21.184	1.00	43.83
MOTA	225	CB	VAL	1492	4.680	9.244	20.709	1.00	41.60
MOTA	226	CG1	VAL	1492	4.138	7.849	20.937	1.00	41.35
ATOM	227	CG2	VAL	1492	5.007	9.445	19.237	1.00	42.72
ATOM	228	С	VAL	1492	3.458	10.084	22.683	1.00	44.45
ATOM	229	0	VAL	1492	4.335	10.437	23.482	1.00	43.86
ATOM	230	N	VAL	1493	2.309	9.548	23.070	1.00	42.67
ATOM	232	CA	VAL	1493	2.029	9.321	24.477	1.00	41.05
MOTA	233	CB	VAL	1493	0.884	10.242	25.013	1.00	40.64
ATOM	234	CG1	VAL	1493	1.177	11.693	24.722	1.00	42.40
MOTA	235	CG2	VAL	1493	-0.459	9.844	24.427	1.00	43.36
MOTA	236	C	VAL		1.626	7.880		1.00	40.09
ATOM	237	0	VAL	1493	1.129	7.212	23.796	1.00	39.99
ATOM	238	N	LEU	1494	1.927	7.374	25.890	1.00	37.10
ATOM	240	CA	LEU	1494	1.535	6.036	26.250	1.00	35.08
MOTA	241	CB	LEU	1494	2.359	5.542	27.440	1.00	35.57
ATOM	242	CG	LEU	1494	2.036	4.161	28.007	1.00	36.87
ATOM	243	CD1	LEU	1494	2.123	3.085	26.931	1.00	36.90
MOTA	244	CD2	LEU	1494	2.998	3.860	29.143	1.00	41.99
MOTA	245	C	LEU	1494	0.077	6.236	26.648	1.00	33.31
ATOM	246	0	LEU	1494	-0.311	7.318	27.097	1.00	32.93
MOTA	247	N	ALA	1495	-0.740	5.219	26.435	1.00	33.35
MOTA	249	CA	ALA	1495	-2.147	5.292	26.773	1.00	30.67
MOTA	250	CB	ALA	1495	-2.923	5.937		1.00	30.35
MOTA	251	С	ALA	1495	-2.661	3.893	27.025	1.00	29.97

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MOTA 252 0 ALA 1495 -1.944 2.909 26.840 1.00 28.15 **ATOM** 253 1496 30.37 N GLU -3.898 3.813 27.488 1.00 MOTA 255 -4.537 CA GLU 1496 2.536 27.745 1.00 31.47 **ATOM** 256 CB GLU 1496 -4.862 2.392 29.223 1.00 32.48 MOTA 257 CG GLU 1496 -3.627 2.239 30.093 1.00 37.81 MOTA 258 CD GLU 1496 -3.938 2.426 31.565 1.00 41.09 MOTA 259 OE1 GLU 1496 -4.328 3.548 31.944 1.00 41.53 MOTA 260 OE2 **GLU** 1496 -3.797 1.453 32.341 44.12 1.00 MOTA 261 C GLU 1496 -5.806 2.524 26.916 1.00 32.72 ATOM 262 O GLU 1496 -6.586 3.478 26.954 1.00 33.91 ATOM 263 N ALA 1497 -5.953 1.494 26.094 1.00 31.06 MOTA 265 CA ALA 1497 -7.117 1.353 25.239 1.00 32.33 MOTA 266 CB 1497 ALA -6.691 0.879 23.859 1.00 29.56 MOTA 267 С ALA 1497 -8.056 0.343 25.885 1.00 32.26 MOTA 268 0 ALA 1497 -7.648 -0.773 26.197 1.00 33.55 MOTA 269 N ILE 1498 -9.286 0.759 26.160 1.00 32.99 MOTA 271 CA ILE 1498 -10.276-0.126 26.766 1.00 34.00 MOTA 272 CB ILE 1498 -11.329 0.668 27.592 1.00 34.69 ATOM 273 CG2 ILE 1498 -12.341 -0.288 28.240 1.00 34.24 **ATOM** 274 CG1 ILE 1498 -10.647 1.496 28.686 33.56 1.00 ATOM 275 CD1 ILE 1498 -11.543 2.572 1.00 29.258 31.25 **ATOM** 276 C ILE 1498 -10.994 -0.830 25.624 1.00 35.71 **ATOM** 277 O ILE 1498 -11.618 -0.181 24.786 1.00 34.88 MOTA 278 N GLY 1499 -10.890 -2.147 25.573 1.00 40.43 **ATOM** 280 CA GLY 1499 -11.553 -2.884 24.516 1.00 47.63 MOTA 281 C GLY 1499 -10.670 -3.233 23.330 1.00 53.08 ATOM 282 GLY 0 1499 -9.934 -4.226 23.380 1.00 54.97 ATOM 283 N LEU 1500 -10.713 -2.394 22.294 1.00 54.18 ATOM 285 CA LEU 1500 -9.957 -2.603 21.055 1.00 55.26 MOTA 286 CB LEU 1500 -8.444 -2.726 21.305 1.00 55.39 MOTA 287 -7.562 CG LEU 1500 -1.472 1.00 21.241 54.27 **ATOM** 288 CDI LEU 1500 -6.110 -1.891 21.367 1.00 52.89 **ATOM** 289 CD2 LEU 1500 -7.768 -0.711 19.935 1.00 50.91 ATOM 290 C LEU 1500 -10.453 -3.830 20.288 1.00 55.39 MOTA 291 O LEU 1500 -10.376 -4.963 20.774 1.00 56.23 **ATOM** 292 N PRO 1505 -13.315 -5.836 25.394 1.00 53.03 **ATOM** 293 CDPRO 1505 -13.945 -7.14825.167 1.00 55.12 **ATOM** 294 CA PRO 1505 -14.306 -4.848 25.846 1.00 50.62 **ATOM** 295 CBPRO 1505 -15.635 -5.607 25.715 1.00 50.09 **MOTA** 296 CG **PRO** 1505 -15.241-7.031 25.950 1.00 52.18 **ATOM** 297 C PRO 1505 -14.039 -4.348 27.273 1.00 46.35 MOTA 298 O PRO 1505 -14.065 -3.143 27.524 1.00 45.82 **ATOM** 299 N ASN 1506 -13.711 -5.261 28.181 1.00 42.76 **ATOM** 301 CA asn 1506 -13.433-4.892 29.566 1.00 45.29 **ATOM** 302 CB ASN 1506 -14.283 -5.728 30.529 1.00 45.92 ATOM 303 CG ASN 1506 -15.752 -5.395 30.441 1.00 46.17 MOTA 304 OD1 ASN 1506 -16.132 -4.232 30.390 1.00 48.57 MOTA 305 ND2 1506 ASN -16.589 -6.418 30.406 1.00 48.63 MOTA 308 C ASN 1506 -11.954 -5.008 29.939 1.00 45.33 MOTA 309 0 ASN 1506 -11.597 -5.084 31.121 1.00 44.53 MOTA 310 N ARG 1507 -11.100 -5.010 28.924 1.00 45.63 MOTA 312 CA ARG 1507 -9.660 -5.122 29.117 1.00 45.57 ATOM 313 CB ARG 1507 -9.131 -6.354 28.375 1.00 53.33 **ATOM** 314 CG ARG 1507 -9.407 -7.685 29.043 1.00 61.39

ATOM	315	CD	ARG	1507	-8.336	-8.028	30.063	1.00	67.74
MOTA	316	NE	ARG	1507	-8.525	-9.376	30.585	1.00	74.64
MOTA	318	CZ	ARG	1507	-7.970	-9.842	31.701	1.00	80.01
MOTA	319	NHl	ARG	1507	-7.166	-9.075	32.433	1.00	80.04
MOTA	322	NH2	ARG	1507	-8.268	-11.068	32.115	1.00	83.41
ATOM	325	С	ARG	1507	-8.964	-3.897	28.555	1.00	40.94
ATOM	326	0	ARG	1507	-9.370	-3.375	27.517	1.00	37.60
ATOM	327	N	VAL	1508	-7.956	-3.409	29.267	1.00	39.33
ATOM	329	CA	VAL	1508	-7.190	-2.269	28.789	1.00	37.26
MOTA	330	СВ	VAL	1508	-6.854	-1.224	29.905	1.00	36.25
ATOM	331	CG1	VAL	1508	-8.124	-0.739	30.571	1.00	39.63
MOTA	332	CG2	VAL	1508	-5.903	-1.796	30.928	1.00	36.92
ATOM	333	C ,	VAL	1508	-5.898	-2.818	28.188	1.00	34.38
ATOM	334	0	VAL	1508		-3.851	28.630	1.00	32.85
ATOM	335	N	THR	1509	-5.406	-2.140	27.159	1.00	
ATOM	337	CA	THR	1509	-4.174	-2.523	26.491	1.00	30.47
ATOM	338	СВ	THR	1509	-4.455	-2.959	25.027	1.00	31.65 34.13
ATOM	339	OG1	THR	1509	-5.426	-4.013	25.027	1.00	
ATOM	341	CG2	THR	1509	-3.184	-3.458	24.345	1.00	40.74
ATOM	342	C	THR	1509	-3.270	-1.299	26.461	1.00	31.06
ATOM	343	0	THR	1509	-3.716	-0.219			28.38
ATOM	344	N	LYS	1510	-2.023		26.104	1.00	27.78
ATOM	346	CA	LYS	1510	-1.101	-1.442	26.896	1.00	29.48
ATOM	347	CB	LYS	1510		-0.312	26.835	1.00	30.54
ATOM	348	CG	LYS	1510	0.172 -0.037	-0.558 -0.600	27.635	1.00	27.88
ATOM	349	CD	LYS	1510	1.284		29.118	1.00	33.91
ATOM	350	CE	LYS	1510	1.145	-0.759	29.840	1.00	40.30
ATOM	351	NZ	LYS	1510		-1.674	31.062	1.00	46.24
ATOM	355	C	LYS	1510	0.338	-1.096	32.187	1.00	49.09
ATOM	356	0	LYS	1510	-0.757	-0.166	25.365	1.00	28.64
ATOM	357	N	VAL	1511	-0.402	-1.142	24.704	1.00	28.76
ATOM	359	CA	VAL	1511	-0.902 -0.627	1.048 1.347	24.856	1.00	29.34
ATOM	360	СВ	VAL	1511			23.463	1.00	29.79
ATOM	361	CG1	VAL	1511	-1.951 -2.681	1.457	22.658	1.00	27.14
ATOM	362	CG2	VAL	1511	-2.837	0.111 2.561	22.657 23.243	1.00	24.56
ATOM	°363	C	VAL	1511	0.123	2.672		1.00	22.15
ATOM	364	0	VAL	1511	0.213	3.413	23.361	1.00	29.83
ATOM	365	N	ALA	1512	0.705	2.939	24.338	1.00	33.14
ATOM	367	CA	ALA	1512	1.405	4.192	22.196	1.00	27.86
ATOM	368	CB	ALA	1512	2.743		21.962	1.00	25.55
ATOM	369	C	ALA	1512	0.500	3.935 5.009	21.297	1.00	24.69
ATOM	370	0	ALA	1512	-0.061	4.483	21.057 20.107	1.00	25.25
ATOM	371	N	VAL	1513	0.340	6.289		1.00	27.18
ATOM	373	CA	VAL	1513			21.360	1.00	29.63
ATOM	374	CB	VAL		-0.520	7.165	20.573	1.00	32.66
ATOM				1513	-1.704	7.713	21.422	1.00	32.47
	375 376	CG1	VAL	1513	-2.609	8.585	20.574	1.00	32.29
MOTA	376	CG2	VAL	1513	-2.508	6.559	22.031	1.00	32.15
MOTA	377	C	VAL	1513	0.238	8.334	19.938	1.00	34.67
ATOM	378	0	VAL	1513	0.792	9.185	20.635	1.00	34.65
ATOM	379	N	LYS	1514	0.207	8.367	18.605	1.00	36.88
ATOM	381	CA	LYS	1514	0.859	9.390	17.789	1.00	36.43
ATOM	382	CB	LYS	1514	1.349	8.764	16.489	1.00	36.37
MOTA	383	CG	LYS	1514	2.250	7.563	16.697	1.00	39.49
MOTA	384	CD	LYS	1514	2.559	6.854	15.390	1.00	45.29

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MOTA	385	CE	LYS	1514	3.080	7.815	14.331	1.00	50.70
ATOM	386	NZ	LYS	1514	4.212	8.685	14.798	1.00	51.41
ATOM	390	C	LYS	1514	-0.121	10.496	17.459	1.00	36.75
ATOM	391	0	LYS	1514	-1.228	10.234	16.978	1.00	35.42
MOTA	392	N	MET	1515	0.294	11.731	17.700	1.00	38.12
MOTA	394	CA	MET	1515	-0.545	12.882	17.432	1.00	41.90
MOTA	395	СВ	MET	1515	-1.371	13.238	18.668	1.00	43.08
MOTA	396	CG	MET	1515	-0.536	13.601	19.880	1.00	45.01
MOTA	397	SD	MET	1515	-1.561	13.784	21.324	1.00	46.03
ATOM	398	CE	MET	1515	-1.675	12.072	21.885	1.00	44.02
ATOM	399	С	MET	1515	0.314	14.065	17.021	1.00	44.65
ATOM	400	0	MET	1515	1.543	14.013	17.094	1.00	45.64
MOTA	401	N	LEU	1516	-0.347	15.123	16.568	1.00	47.08
ATOM	403	CA	LEU	1516	0.329	16.337	16.134	1.00	48.08
ATOM	404	CB	LEU	1516	-0.500	17.033	15.054	1.00	45.50
ATOM	405	CG	LEU	1516	-0.764	16.265	13.764	1.00	43.22
ATOM	406	CD1	LEU	1516	-1.783	17.014	12.946	1.00	40.32
MOTA	407	CD2	LEU	1516	0.540	16.072	12.991	1.00	43.78
MOTA	408	С	LEU	1516	0.516	17.302	17.297	1.00	51.27
ATOM	409	0	LEU	1516	-0.214	17.249	18.291	1.00	50.37
ATOM	410	N	LYS	1517	1.491	18.191	17.157	1.00	55.47
MOTA	412	CA	LYS	1517	1.757	19.207	18.168	1.00	59.10
MOTA	413	CB	LYS	1517	3.203	19.702	18.068	1.00	61.61
ATOM	414	CG	LYS	1517	4.251	18.669	18.462	1.00	64.82
ATOM	415	CD	LYS	1517	5.635	19.109	18.018	1.00	67.42
ATOM	416	CE	LYS	1517	6.696	18.102	18.432	1.00	71.76
ATOM	417	NZ	LYS	1517	8.021	18.411	17.812	1.00	73.57
ATOM	421	С	LYS	1517	0.794	20.365	17.920	1.00	59.91
ATOM	422	0	LYS	1517	0.187	20.456	16.852	1.00	59.88
ATOM	423	N	SER	1518	0.686	21.267	18.886	1.00	61.85
MOTA	425	CA	SER	1518	-0.216	22.409	18.760	1.00	63.70
MOTA	426	CB	SER	1518	-0.158	23.274	20.024	1.00	64.21
ATOM	427	С	SER	1518	0.079	23.263	17.529	1.00	64.37
ATOM	428	0	SER	1518	-0.841	23.757	16.875	1.00	66.16
ATOM	429	N	ASP	1519	1.359	23.410	17.202	1.00	64.15
ATOM	431	CA	ASP	1519	1.767	24.217	16.054	1.00	64.55
MOTA	432	CB	ASP	1519	3.109	24.897	16.343	1.00	65.84
ATOM	433	С	ASP	1519	1.858	23.441	14.742	1.00	63.95
MOTA	434	0	ASP	1519	2.432	23.931	13.769	1.00	64.95
MOTA	435	N	ALA	1520	1.303	22.232	14.719	1.00	62.57
MOTA	437	CA	ALA	1520	1.329	21.398	13.521	1.00	60.34
MOTA	438	CB	ALA	1520	0.704	20.039	13.810	1.00	60.53
MOTA	439	С	ALA	1520	0.616	22.062	12.353	1.00	58.21
MOTA	440	0	ALA	1520	-0.464	22.631	12.506	1.00	58.32
ATOM	441	N	THR	1521	1.241	22.001	11.186	1.00	55.96
ATOM	443	CA	THR	1521	0.673	22.582	9.981	1.00	54.98
ATOM	444	CB	THR	1521	1.783	23.013	9.031	1.00	53.84
MOTA	445	OG1	THR	1521	2.554	21.862	8.659	1.00	55.84
MOTA	447	CG2	THR	1521	2.693	24.026	9.703	1.00	55.01
ATOM	448	C	THR	1521	-0.184	21.545	9.261	1.00	54.25
MOTA	449	0	THR	1521	-0.190	20.371	9.629	1.00	54.74
ATOM	450	N	GLU	1522	-0.877	21.974	8.212	1.00	53.32
ATOM	452	CA	GLU	1522	-1.702	21.066	7.423	1.00	52.64
ATOM	453	СВ	GLU	1522	-2.472	21.829	6.339	1.00	53.55
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ATOM	454	С	GLU	1522	-0.793	20.012	6.780	1.00	51.95
MOTA	455	0	GLU	1522	-1.226	18.895	6.504	1.00	53.28
ATOM	456	N	LYS	1523	0.464	20.377	6.544	1.00	48.66
ATOM	458	CA	LYS	1523	1.429	19.460	5.963	1.00	46.30
ATOM	459	CB	LYS	1523	2.730	20.201	5.620	1.00	48.30
ATOM	460	CG	LYS	1523	3.889	19.308	5.164	1.00	49.58
ATOM	461	CD	LYS	1523	3.487	18.388	4.016	1.00	50.87
MOTA	462	CE	LYS	1523	4.688	17.635	3.466	1.00	54.08
ATOM	463	NZ	LYS	1523	4.271	16.629	2.440	1.00	57.87
ATOM	467	С	LYS	1523	1.699	18.391	7.006	1.00	43.89
ATOM	468	0	LYS	1523	1.747	17.202	6.697	1.00	43.92
ATOM	469	N	ASP	1524	1.857	18.828	8.249	1.00	42.71
MOTA	471	CA	ASP	1524	2.114	17.915	9.351	1.00	42.11
ATOM	472	CB	ASP	1524	2.313	18.701	10.653	1.00	44.94
MOTA	473	CG	ASP	1524	3.623	19.490	10.673	1.00	48.90
MOTA	474	OD1	ASP	1524	3.692	20.512	11.392	1.00	51.88
ATOM	475	OD2	ASP	1524	4.590	19.084	9.990	1.00	50.06
ATOM	476	С	ASP	1524	0.956	16.931	9.481	1.00	39.85
MOTA	477	0	ASP	1524	1.164	15.738	9.748	1.00	39.01
MOTA	478	N	LEU	1525	-0.261	17.438	9.296	1.00	38.32
ATOM	480	CA	LEU	1525	-1.461	16.610	9.355	1.00	36.16
ATOM	481	CB	LEU	1525	-2.720	17.470	9.200	1.00	35.13
ATOM	482	CG	LEU	1525	-4.081	16.760	9.186	1.00	34.70
MOTA	483	CD1	LEU	1525	-4.184	15.668	10.252	1.00	36.15
ATOM	484	CD2	LEU	1525	-5.162	17.789	9.395	1.00	32.96
ATOM	485	С	LEU	1525	-1.406	15.560	8.254	1.00	34.31
MOTA	486	0	LEU	1525	-1. 57 5	14.377	8.518	1.00	33.34
MOTA	487	N	SER	1526	-1.136	16.005	7.030	1.00	36.40
ATOM	489	CA	SER	1526	-1.039	15.128	5.865	1.00	37.16
ATOM	490	CB	SER	1526	-0.669	15.931	4.618	1.00	38.84
MOTA	491	OG	SER	1526	-1.736	16.779	4.245	1.00	49.61
ATOM	493	С	SER	1526	-0.021	14.016	6.044	1.00	35.90
ATOM	494	0	SER	1526	-0.273	12.873	5.670	1.00	36.68
MOTA	495	N	ASP	1527	1.142	14.349	6.591	1.00	35.89
MOTA	497	CA	ASP	1527	2.177	13.342	6.796	1.00	35.25
ATOM	498	CB	ASP	1527	3.497	13.998	7.201	1.00	35.58
ATOM	499	CG	ASP	1527	4.100	14.850	6.081	1.00	37.19
ATOM	500	OD1	ASP	1527	3.750	14.653	4.895	1.00	37.38
ATOM	501	OD2	ASP	1527	4.932	15.726	6.395	1.00	42.93
ATOM	502	С	ASP	1527	1.749	12.274	7.799	1.00	31.77
ATOM	503	0	ASP	1527	2.000	11.090	7.594	1.00	30.58
ATOM	504	N	LEU	1528	1.055	12.684	8.853	1.00	31.80
ATOM	506	CA	LEU	1528	0.581	11.730	9.857	1.00	33.53
ATOM	507	CB	LEU	1528	-0.002	12.471	11.076	1.00	32.20
ATOM	508	CG	LEU	1528	-0.440	11.623	12.275	1.00	32.63
MOTA	509	CD1	LEU	1528	0.705	10.708	12.709	1.00	33.09
ATOM	510		LEU	1528	-0.891	12.512	13.426	1.00	31.52
ATOM	511	С	LEU	1528	-0.468	10.792	9.235	1.00	32.89
ATOM	512	0	LEU	1528	-0.494	9.589	9.521	1.00	32.39
ATOM	513	N	ILE	1529	-1.336	11.357	8.393	1.00	33.72
ATOM	515	CA	ILE	1529	-2.376	10.591	7.711	1.00	30.48
ATOM	516	CB	ILE	1529	-3.336	11.505	6.895	1.00	28.85
MOTA	517	CG2	ILE	1529	-4.229	10.662	5.997	1.00	28.54
MOTA	518	CG1	ILE	1529	-4.200	12.344	7.843	1.00	29.52

MOTA	519	CD1	ILE	1529	-5.143	13.308	7.133	1.00	32.07
MOTA	520	C	ILE	1529	-1.698	9.608	6.768	1.00	31.50
MOTA	521	0	ILE	1529	-2.009	8.419	6.780	1.00	30.75
ATOM	522	N	SER	1530	-0.749	10.100	5.974	1.00	33.28
ATOM	524	CA	SER	1530	-0.011	9.250	5.038	1.00	32.48
MOTA	525	CB	SER	1530	1.114	10.042	4.368	1.00	37.20
MOTA	526	OG	SER	1530	0.604	11.218	3.766	1.00	49.93
MOTA	528	C	SER	1530	0.583	8.045	5.756	1.00	29.05
ATOM	529	0	SER	1530	0.397	6.909	5.316	1.00	28.66
MOTA	530	N	GLU	1531	1.259	8.290	6.878	1.00	28.21
MOTA	532	CA	GLU	1531	1.880	7.207	7.631	1.00	27.30
MOTA	533	CB	GLU	1531	2.656	7.733	8.839	1.00	28.90
MOTA	534	CG	GLU	1531	3.271	6.609	9.672	1.00	27.17
MOTA	535	ന	GLU	1531	4.047	7.081	10.886	1.00	30.07
ATOM	536	OE1	GLU	1531	4.779	6.244	11.448	1.00	34.78
MOTA	537	OE2	GLU	1531	3.931	8.256	11.291	1.00	31.96
MOTA	538	C	GLU	1531	0.870	6.162	8.072	1.00	27.73
MOTA	539	0	GLU	1531	1.160	4.961	8.028	1.00	28.72
MOTA	540	N	MET	1532	-0.286	6.621	8.555	1.00	29.78
ATOM	542	CA	MET	1532	-1.373	5.734	8.990	1.00	28.79
ATOM	543	CB	MET	1532	-2.501	6.553	9.646	1.00	28.90
MOTA MOTA	544	CC	MET	1532	-3.763	5.741	9.993	1.00	29.73
ATOM	545 546	SD CE	MET	1532	-5.089	6.693	10.765	1.00	30.19
ATOM	547	CE	MET MET	1532 1532	-5.455	7.870	9.494	1.00	26.70
ATOM	548	0	MET	1532	-1.935 -2.166	4.937	7.796	1.00	28.34
ATOM	549	N	GLU	1533	-2.166 -2.165	3.730 5.624	7.893	1.00	26.62
ATOM	551	CA	GLU	1533	-2.684	4.984	6.678 5.467	1.00 1.00	28.85
ATOM	552	СВ	GLU	1533	-2.936	6.027	4.384	1.00	28.24 25.42
ATOM	553	CG	GLU	1533	-4.099	6.956	4.719	1.00	30.05
ATOM	554	CD	GLU	1533	-5.393	6.201	5.021	1.00	29.47
ATOM	555	OE1	GLU	1533	-5.794	5.336	4.211	1.00	29.01
MOTA	556	OE2	GLU	1533	~6.011	6.472	6.073	1.00	33.98
ATOM	557	С	GLU	1533	-1.694	3.944	4.968	1.00	28.01
MOTA	558	0	GLU	1533	-2.072	2.845	4.573	1.00	27.39
MOTA	559	N	MET	1534	-0.416	4.293	5.036	1.00	29.06
ATOM	561	CA	MET	1534	0.662	3.413	4.621	1.00	29.74
MOTA	562	CB	MET	1534	1.992	4.155	4.755	1.00	33.16
ATOM	563	CG	MET	1534	3.198	3.270	4.682	1.00	42.88
ATOM	564	SD	MET	1534	3.805	3.127	3.042	1.00	50.20
MOTA	565	CE	MET	1534	5.137	4.169	3.159	1.00	42.64
MOTA	566	С	MET	1534	0.641	2.156	5.493	1.00	26.90
ATOM	567	0	MET	1534	0.755	1.038	4.990	1.00	27.05
ATOM	568	N	MET	1535	0.512	2.348	6.803	1.00	25.42
MOTA	570	CA	MET	1535	0.437	1.233	7.737	1.00	25.88
MOTA	571	CB	MET	1535	0.325	1.741	9.181	1.00	27.63
ATOM	572	CG	MET	1535	1.607	2.391	9.737	1.00	27.26
ATOM	573	SD	MET	1535	1.584	2.561	11.564	1.00	29.49
ATOM	574	CE	MET	1535	1.294	4.255	11.699	1.00	28.22
ATOM	575	C	MET	1535	-0.754	0.324	7.396	1.00	26.28
ATOM	576	0	MET	1535	-0.645	-0.908	7.469	1.00	25.93
ATOM	577	N	LYS	1536	-1.890	0.928	7.032	1.00	27.19
ATOM	579	CA	LYS	1536	-3.087	0.162	6.647	1.00	27.20
MOTA	580	CB	LYS	1536	-4.257	1.088	6.310	1.00	25.29

MOTA	581	CG	LYS	1536	-4.897	1.770	7.491	1.00	23.86
ATOM	582	CD	LYS	1536	-5.884	2.820	7.017	1.00	22.16
MOTA	583	CE	LYS	1536	-6.460	3.588	8.174	1.00	22.25
MOTA	584	NZ	LYS	1536	-7.484	4.541	7.713	1.00	23.40
ATOM	588	C	LYS	1536	-2.785	-0.699	5.423	1.00	24.52
MOTA	589	0	LYS	1536	-3.069	-1.889	5.403	1.00	26.61
ATOM	590	N	MET	1537	-2.183	-0.093	4.411	1.00	27.12
MOTA	59 2	CA	MET	1537	-1.843	-0.815	3.194	1.00	28.06
ATOM	593	CB	MET	1537	-1.269	0.147	2.147	1.00	30.36
MOTA	594	CG	MET	1537	-2.265	1.164	1.591	1.00	36.31
ATOM	595	SD	MET	1537	-3.699	0.444	0.727	1.00	42.19
MOTA	596	CE	MET	1537	-2.912	-0.057	-0.793	1.00	36.22
MOTA	597	C	MET	1537	-0.857	-1.952	3.447	1.00	26.98
- ATOM	598	O -	MET	1537	-1.060	-3.065	2.963	1.00	25:34
MOTA	599	N	ILE	1538	0.188	-1.678	4.229	1.00	27.69
ATOM	601	CA	ILE	1538	1.234	-2.674	4.535	1.00	25.39
ATOM	602	CB	ILE	1538	2.454	-2.006	5.255	1.00	24.42
MOTA	603	CG2	ILE	1538	3.424	-3.051	5.811	1.00	25.28
MOTA	604	CG1	ILE	1538	3.223	-1.131	4.269	1.00	23.88
MOTA	605	CD1	ILE	1538	4.373	-0.372	4.901	1.00	27.19
MOTA	606	C	ILE	1538	0.760	-3.922	5.292	1.00	25.59
MOTA	607	0	ILE	1538	1.242	-5.033	5.035	1.00	26.11
MOTA	608	N	GLY	1539	-0.193	-3.767	6.208	1.00	26.13
MOTA	610	CA	GLY	1539	-0.661	-4.940	6.934	1.00	25.25
ATOM	611	С	GLY	1539	0.191	-5.280	8.149	1.00	26.77
ATOM	612	0	GLY	1539	1.214	-4.637	8.414	1.00	25.42
MOTA	613	N	LYS	1540	-0.204	-6.327	8.862	1.00	25.62
MOTA	615	CA	LYS	1540	0.467	-6.716	10.092	1.00	26.38
ATOM	616	CB	LYS	1540	-0.552	-7.283	11.084	1.00	27.15
ATOM	617	CG	LYS	1540	-1.573	-6.303	11.550	1.00	34.23
MOTA	618	CD	LYS	1540	-2.528	-6.943	12.546	1.00	40.69
ATOM	619	CE	LYS	1540	-3.559	-5.927	13.057	1.00	44.08
MOTA	620	NZ	LYS	1540	-2.956	-4.800	13.833	1.00	44.05
MOTA	624	С	LYS	1540	1.609	-7.705	10.014	1.00	24.37
ATOM	625	0	LYS	1540	1.627	-8.600	9.181	1.00	26.12
ATOM	626	N	HIS	1541	2.545	-7.538	10.936	1.00	24.41
ATOM	628	CA	HIS	1541	3.666	-8.440	11.091	1.00	25.41
MOTA	629	СВ	HIS	1541	4.772	-8.228	10.057	1.00	21.88
ATOM	630	CG	HIS	1541	5.798	-9.320	10.068	1.00	22.68
MOTA	631	CD2	HIS	1541	5.823	-10.522	9.444	1.00	21.40
ATOM	632	ND1	HIS	1541	6.939	-9.268	10.843	1.00	22.12
MOTA	634	CE1	HIS	1541	7.619	-10.389	10.697	1.00	24.78
ATOM	635	NE2	HIS	1541	6.966	-11.167	9.854	1.00	27.00
ATOM	637	c /	HIS	1541	4.234	-8.328	12.494	1.00	25.47
MOTA	638	0	HIS	1541	4.364	-7.239	13.050	1.00	26.77
ATOM	639	N	LYS	1542	4.560	-9.476	13.063	1.00	26.38
ATOM	641	CA	LYS	1542	5.127	-9.552	14.401	1.00	30.07
ATOM	642	CB	LYS	1542	5.515	-11.003	14.692	1.00	31.38
ATOM	643	CG	LYS	1542	6.061	-11.252	16.077	1.00	42.79
MOTA	644	CD	LYS	1542	6.289	-12.735	16.294	1.00	50.84
MOTA	645	CE	LYS	1542	7.041	-13.374	15.114	1.00	56.75
ATOM	646	NZ	LYS	1542	7.511	-14.763	15.424	1.00	61.29
ATOM	650	C	LYS	1542	6.342	-8.652	14.624	1.00	27.65
ATOM	651	0	LYS	1542	6.519	-8.113	15.711	1.00	26.83

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MOTA	652	N	ASN	1543	7.146	-8.445	13.585	1.00	27.20
ATOM	654	CA	ASN	1543	8.354	-7.642	13.735	1.00	25.50
MOTA	655	CB	ASN	1543	9.578	-8.431	13.260	1.00	25.59
ATOM	656	CG	ASN	1543	9.712	-9.767	13.974	1.00	22.64
MOTA	657	OD1	asn	1543	9.522	-10.821	13.371	1.00	26.76
ATOM	658	ND2	ASN	1543	9.970	-9.727	15.273	1.00	25.56
ATOM	661	С	ASN	1543	8.374	-6.213	13.226	1.00	25.48
ATOM	662	0	ASN	1543	9.417	-5.692	12.842	1.00	24.58
ATOM	663	N	ILE	1544	7.209	-5.575	13.244	1.00	24.60
MOTA	665	CA	ILE	1544	7.065	-4.177	12.868	1.00	22.32
MOTA	666	CB	ILE	1544	6.524	-3.972	11.409	1.00	25.82
MOTA	667	CG2	ILE	1544	7.401	-4.720	10.403	1.00	24.24
ATOM	668	CG1	ILE	1544	5.057	-4.411	11.279	1.00	26.04
MOTA	669	CD1	ILE	1544	4.446	-4.121	9.901	1.00	23.20
MOTA	670	С	ILE	1544	6.075	-3.598	13.881	1.00	22.37
ATOM	671	0	ILE	1544	5.364	-4.345	14.559	1.00	21.68
ATOM	672	N	ILE	1545	6.111	-2.290	14.076	1.00	23.72
ATOM	674	CA	ILE	1545	5.169	-1.650	14.989	1.00	25.92
MOTA	675	CB	ILE	1545	5.602	-0.199	15.364	1.00	27.24
ATOM	676	CG2	ILE	1545	4.452	0.554	16.035	1.00	22.76
ATOM	677	CG1	ILE	1545	6.839	-0.219	16.285	1.00	25.57
ATOM	678	CD1	ILE	1545	6.591	-0.797	17.686	1.00	24.66
ATOM	679	C	ILE	1545	3.877	-1.612	14.179	1.00	26.03
MOTA	680	0	ILE	1545	3.823	-0.988	13.122	1.00	25.70
ATOM	681	N	ASN	1546	2.849	-2.293	14.669	1.00	24.79
MOTA	683	CA	ASN	1546	1.577	-2.354	13.956	1.00	25.51
ATOM	684	CB	ASN	1546	0.922	-3.727	14.137	1.00	25.17
ATOM	685	CG	ASN	1546	1.730	-4.839	13.539	1.00	21.67
ATOM	686	OD1	ASN	1546	1.856	-4.947	12.329	1.00	24.29
ATOM	687	ND2	ASN	1546	2.278	-5.686	14.384	1.00	22.24
MOTA	690	C	ASN	1546	0.578	-1.276	14.349	1.00	26.85
ATOM	691	0	ASN	1546	0.630	-0.724	15.453	1.00	28.67
ATOM	692	N	LEU	1547	-0.301	-0.956	13.407	1.00	27.70
ATOM	694	CA	LEU	1547	-1.357	0.019	13.622	1.00	27.64
ATOM	695	СВ	LEU	1547	-1.945	0.481	12.284	1.00	24.87
MOTA	696	CG	LEU	1547	-3.173	1.400	12.337	1.00	23.25
ATOM	697	CD1	LEU	1547	-2.790	2.763	12. 9 29	1.00	23.76
ATOM	698	CD2	LEU	1547	-3.757	1.569	10.923	1.00	23.47
ATOM	699	C	LEU	1547	-2.415	-0.771	14.396	1.00	27.27
ATOM	700	0	LEU	1547	-2.663	-1.952	14.103	1.00	25.27
MOTA	701	N	LEU	1548	-3.000	-0.130	15.400	1.00	27.94
MOTA	703	CA	LEU	1548	-4.017	-0.770	16.223	1.00	26.98
MOTA	704	CB	LEU	1548	-3.623	-0.735	17.708	1.00	24.65
MOTA	705	CG	LEU	1548	-2.327	-1.450	18.108	1.00	25.38
ATOM	706	CD1	LEU	1548	-2.189	-1.428	19.613	1.00	25.73
ATOM	707	CD2	LEU	1548	-2.337	-2.886	17.621	1.00	23.92
ATOM	708	C	LEU	1548	-5.369	-0.113	16.042	1.00	26.65
ATOM	709	0	LEU	1548	-6.392	-0.752	16.238	1.00	27.11
ATOM	710	N	GLY	1549	-5.378	1.163	15.684	1.00	25.04
ATOM	712	CA	GLY	1549	-6.643	1.855	15.516	1.00	25.47
ATOM	713	C	GLY	1549	-6.417	3.336	15.367	1.00	26.23
ATOM	714	0	GLY	1549	-5.267	3.781	15.287	1.00	28.41
ATOM	715	N	ALA	1550	-7.501	4.104	15.349	1.00	25.49
MOTA	717	CA	ALA	1550	-7.408	5.550	15.198	1.00	24.81

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MOTA 718 CB ALA 1550 -7.176 5.913 13.724 1.00 21.79 MOTA 719 С ALA 1550 -8.645 6.271 15.691 1.00 25.51 **ATOM** 720 0 ALA 1550 -9.738 5.702 15.726 1.00 24.09 **ATOM** 721 N CYS 1551 -8.440 7.527 16.080 1.00 24.90 **MOTA** 723 CA CYS 1551 -9.492 8.438 16.511 1.00 26.80 MOTA 724 CB CYS 1551 -9.243 8.932 17.944 1.00 26.32 MOTA 725 SG CYS 1551 -9.333 7.655 19.223 1.00 32.31 **ATOM** 726 CYS 1551 -9.341 C 9.585 15.502 1.00 28.31 MOTA 727 CYS 1551 -8.361 0 10.338 15.537 1.00 28.42 **MOTA 728** N THR 1552 -10.261 9.660 14.547 1.00 28.38 **ATOM** 730 THR CA 1552 -10.198 10.671 13.498 1.00 31.26 MOTA 731 CB THR 1552 -10.159 9.977 12.095 1.00 30.07 ATOM 732 THR . OG1 1552 -11.406 9.309 11.836 1.00 29.64 **ATOM** 734 CG2 THR 1552 -9.044 1.00 8.945 12.053 28.65 **ATOM** 735 С THR 1552 -11.355 11.662 13.509 1.00 33.31 **ATOM** 736 THR -11.295 0 1552 12.722 12.874 1.00 31.94 ATOM 737 N GLN 1553 -12.420 11.309 14.214 1.00 36.09 **MOTA** 739 CA GLN 1553 -13.598 12.158 14.245 1.00 39.26 MOTA 740 CB GLN 1553 -14.864 11.299 14.145 1.00 36.61 MOTA 741 CG GLN 1553 -14.932 10.436 12.881 1.00 37.72 MOTA 742 CD GLN 1553 -14.762 11.247 11.601 1.00 38.41 MOTA 743 OE1 GLN 1553 -15.491 12.210 11.363 1.00 37.88 744 MOTA NE2 GLN 1553 -13.798 10.858 10.770 1.00 37.67 MOTA 747 C GLN 1553 -13.671 13.079 15.451 1.00 41.28 MOTA 748 0 GLN 1553 -13.150 12.758 16.513 1.00 41.37 MOTA 749 N ASP 1554 -14.282 14.246 15.243 1.00 44.93 MOTA 48.05 751 CA ASP 1554 -14.487 15.254 16.281 1.00 MOTA 752 CB ASP 1554 -15.828 15.009 16.975 1.00 50.80 MOTA 753 CG ASP 1554 -17.007 15.281 16.067 1.00 56.88 MOTA 754 OD1 ASP 1554 -17.921 16.019 16.491 1.00 63.89 MOTA 755 OD2 ASP 1554 -17.016 14.925 14.776 1.00 58.98 MOTA 756 1554 С ASP -13.367 17.316 15.366 1.00 48.04 **ATOM** 757 **ASP** -13.556 18.502 0 1554 15.056 1.00 48.73 ATOM 758 N GLY 1555 -12.205 15.819 16.860 1.00 44.30 MOTA 760 CA GLY 1555 -11.080 15.960 17.756 1.00 42.32 MOTA 761 С GLY 1555 -9.761 17.052 1.00 15.713 40.69 MOTA 762 GLY 1555 -9.740 0 15.465 15.848 1.00 40.71 MOTA 763 N PRO 1556 -8.644 15.776 17.782 1.00 39.49 MOTA 764 CD PRO 1556 -8.585 15.983 19.235 1.00 40.36 MOTA 765 CA PRO 1556 -7.298 15.566 17.250 1.00 38.37 MOTA 766 CB PRO 1556 -6.405 15.771 18.470 1.00 38.47 MOTA 767 CG PRO 1556 -7.226 16.573 19.388 1.00 41.77 MOTA 768 PRO 1556 -7.140 14.154 16.746 1.00 C 36.92 MOTA 769 0 PRO 1556 -7.606 13.208 17.371 1.00 37.04 **ATOM** 770 N LEU 1557 -6.447 14.017 15.627 1.00 36.70 **MOTA** 772 CA LEU 1557 -6.201 12.719 15.037 1.00 34.81 MOTA 773 CB LEU 1557 -5.528 12.B85 13.664 1.00 32.49 ATOM 774 CG LEU 1557 -5.004 11.623 12.954 1.00 30.83 MOTA 775 LEU 1557 -6.146 CD1 10.655 12.664 1.00 26.28 MOTA 776 CD2 LEU 1557 -4.283 12.014 11.672 1.00 25.55 MOTA 777 1557 LEU -5.290 11.925 15.961 1.00 С 33.63 MOTA 778 LEU 1.00 0 1557 -4.229 12.410 16.369 33.62 **ATOM** 779 N TYR 1558 -5.718 10.724 16.319 1.00 31.97 MOTA 781 1558 -4.902 9.863 17.147 1.00 CA TYR 31.81

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MOTA	782	CB	TYR	1558	-5.614	9.500	18.462	1.00	33.55
ATOM	783	CG	TYR	1558	-5.710	10.638	19.461	1.00	35.33
ATOM	784	CD1	TYR	1558	-6.644	10.608	20.499	1.00	35.68
MOTA	785	CE1	TYR	1558	-6.757	11.670	21.394	1.00	38.60
ATOM	786	CD2	TYR	1558	-4.883	11.759	19.349	1.00	38.62
MOTA	787	CE2	TYR	1558	-4.985	12.824	20.235	1.00	40.33
ATOM	788	CZ	TYR	1558	-5.924	12.781	21.254	1.00	41.70
ATOM	789	OH	TYR	1558	-6.040	13.867	22.104	1.00	42.66
ATOM	791	С	TYR	1558	-4.607	8.604	16.345	1.00	31.08
MOTA	792	0	TYR	1558	-5.527	7.937	15.857	1.00	31.28
MOTA	793	N	VAL	1559	-3.328	8.336	16.116	1.00	28.34
ATOM	795	CA	VAL	1559	-2.934	7.132	15.403	1.00	26.39
ATOM	796	CB	VAL	1559	-1.830	7.401	14.364	1.00	29.17
MOTA	797	CG1	VAL	1559	-1.463	6.103	13.648	1:00	26.25
MOTA	798	CG2	VAL	1559	-2.297	8.461	13.360	1.00	29.56
MOTA	799	C	VAL	1559	-2.411	6.226	16.498	1.00	25.14
ATOM	800	0	VAL	1559	-1.396	6.522	17.120	1.00	28.04
ATOM	801	N	ILE	1560	-3.164	5.171	16.783	1.00	25.28
ATOM	803	CA	ILE	1560	-2.832	4.208	17.831	1.00	24.81
ATOM	804	CB	ILE	1560	-4.133	3.669	18.496	1.00	24.63
ATOM	805	CG2	ILE	1560	-3.790	2.812	19.728	1.00	20.93
ATOM	806	CG1	ILE	1560	-5.044	4.854	18.869	1.00	22.94
MOTA	807	CD1	ILE	1560	-6.499	4.502	19.028	1.00	25.34
ATOM	808	C	ILE	1560	-1.994	3.051	17.286	1.00	26.38
MOTA	809	0	ILE	1560	-2.429	2.301	16.398	1.00	26.14
MOTA	810	N	VAL	1561	~0.782	2.911	17.809	1.00	27.31
MOTA	B12	CA	VAL	1561	0.112	1.852	17.359	1.00	27.32
MOTA	813	CB	VAL	1561	1.309	2.435	16.527	1.00	25.01
ATOM	814	CG1	VAL	1561	0.785	3.220	15.338	1.00	19.39
ATOM	815	CG2	VAL	1561	2.170	3.340	17.397	1.00	26.08
ATOM	816	С	VAL	1561	0.615	1.029	18.548	1.00	25.89
MOTA	817	0	VAL	1561	0.364	1.373	19.713	1.00	25.64
MOTA	818	N	GLU	1562	1.288	-0.076	18.250	1.00	24.49
MOTA	820	CA	GLU	1562	1.806	-0.949	19.284	1.00	25.00
ATOM	821	CB	GLU	1562	2.357	-2.231	18.677	1.00	23.69
ATOM	822	CG	GLU	1562	1.272	-3.170	18.219	1.00	24.29
ATOM	823	CD	GLU	1562	1.814	-4.393	17.514	1.00	27.65
ATOM	824	OE1	GLU	1562	1.218	-5.480	17.649	1.00	29.50
ATOM	825	OE2	GLU	1562	2.832	-4.270	16.807	1.00	32.34
ATOM	826	C	GLU	1562	2.840	-0.279	20.170	1.00	27.27
MOTA	827	0	GLU	1562	3.596	0.576	19.729	1.00	26.18
ATOM	828	N	TYR	1563	2.822	-0.663	21.441	1.00	30.39
ATOM	830	CA	TYR	1563	3.715	-0.121	22.454	1.00	32.48
ATOM	831	СВ	TYR	1563	2.932	0.132	23.750	1.00	33.91
ATOM	832	CG	TYR	1563	3.788	0.535	24.928	1.00	34.93
ATOM	833	CD1	TYR	1563	4.606	1.664	24.871	1.00	34.50
ATOM	834	CE1	TYR	1563	5.374	2.051	25.967	1.00	37.77
ATOM	835	CD2	TYR	1563	3.758	-0.201	26.108	1.00	33.54
MOTA	836	CE2	TYR	1563	4.519	0.171	27.205	1.00	34.94
ATOM	837	CZ	TYR	1563	5.321	1.296	27.128	1.00	37.22
ATOM	838	ОН	TYR	1563	6.087	1.648	28.206	1.00	45.36
ATOM	840	С	TYR	1563	4.896	-1.039	22.730	1.00	31.53
ATOM	841	0	TYR	1563	4.737	-2.252	22.895	1.00	30.43
MOTA	842	N	ALA	1564	6.082	-0.444	22.761	1.00	32.28

ATOM 844 1564 -1.167 CA ALA 7.326 23.026 1.00 32.59 ATOM 845 CB ALA 1564 8.308 -0.957 21.863 1.00 30.11 **ATOM** 846 C ALA 1564 7.897 -0.608 24.334 1.00 31.81 ATOM 847 O ALA 1564 8.563 0.427 24.345 1.00 34.11 **ATOM** 848 N SER 1565 7.619 -1.296 25.434 1.00 34.09 **ATOM** 850 CA SER 1565 8.039 -0.853 26.763 1.00 35.05 MOTA 851 CB SER 1565 7.400 -1.725 27.829 1.00 30.13 **ATOM** 852 OG SER 1565 7.689 -3.084 27.579 1.00 38.17 MOTA 854 C SER 1565 9.526 -0.769 27.041 1.00 35.03 MOTA 855 О SER 1565 9.947 -0.001 27.902 1.00 37.12 **ATOM** 856 N LYS 1566 10.321 -1.557 26.330 1.00 34.55 **ATOM** 858 LYS CA 1566 11.756 -1.559 26.562 1.00 33.48 **MOTA** 859 CB LYS 1566 12.291 -2.990 26.508 1.00 31.90 - - ATOM -860 LYS CG. 1566. 11.674 -3.865 1.00 28.63 27.586 MOTA 861 CD LYS 1566 12.162 -5.287 27.508 1.00 34.97 ATOM 862 CE LYS 1566 11.763 -6.042 28.761 1.00 36.82 MOTA 863 NZ LYS 1566 12.288 -7.433 28.748 1.00 41.32 **ATOM** 867 C LYS 1566 12.567 -0.613 25.691 1.00 34.98 MOTA 868 0 LYS 1566 13.785 -0.740 25.607 1.00 38.03 MOTA 869 N GLY 1567 11.892 0.338 25.049 1.00 36.00 MOTA 871 CA GLY 1567 12.582 1.322 24.222 1.00 34.14 MOTA 872 GLY C 1567 13.245 0.864 22.933 1.00 32.01 MOTA 873 GLY 1567 0 12.975 -0.222 22.439 1.00 31.95 MOTA 874 N ASN 1568 14.091 1.719 22.360 1.00 33.51 ATOM 876 CA ASN 1568 14.774 1.375 21.121 1.00 34.20 MOTA 877 CB ASN 1568 15.203 2.627 20.332 1.00 34.07 MOTA 878 CGASN 1568 16.420 3.321 20.910 1.00 35.09 MOTA 879 OD1 ASN 1568 17.453 2.709 21.156 1.00 34.36 MOTA 880 ND2 ASN 1568 16.317 4.624 21.066 1.00 38.38 **ATOM** 883 C ASN 1568 15.927 0.401 21.325 1.00 33.38 **ATOM** 884 0 ASN 1568 16.490 0.315 22.414 1.00 34.93 MOTA 885 N LEU 1569 16.276 -0.317 20.263 1.00 31.11 **MOTA** 887 CA LEU 1569 17.333 -1.316 20.298 1.00 30.44 MOTA 888 CB LEU 1569 17.437 -2.00B 18.928 1.00 29.46 MOTA 889 LEU 18.741 CG 1569 18.438 -3.148 1.00 29.01 MOTA 890 CD1 LEU 1569 18.285 -4.219 19.840 1.00 28.81 MOTA 18.263 891 CD2 LEU 1569 -3.740 17.338 1.00 26.62 MOTA 892 LEU C 1569 18.706 20.762 -0.805 1.00 30.16 MOTA 893 LEU 1569 О 19.400 -1.501 21.496 1.00 27.32 MOTA 894 N ARG 1570 19.097 0.396 20.344 1.00 30.74 MOTA 896 CA ARG 1570 20.386 0.951 20.758 1.00 33.72 MOTA 897 CB ARG 1570 20.597 2.349 20.160 1.00 32.82 MOTA 898 ARG CG 1570 21.873 3.009 20.662 1.00 36.90 MOTA 899 CD ARG 1570 21.966 4.481 20.332 1.00 39.32 MOTA 900 ARG 1570 NE 20.749 5.222 20.664 1.00 50.32 MOTA 902 CZ ARG 1570 20.376 5.600 21.889 1.00 51.90 MOTA 903 ARG NH1 1570 21.118 5.316 22.960 1.00 50.15 MOTA 906 NH2 ARG 1570 19.246 6.284 22.033 1.00 53.67 909 MOTA C ARG 1570 20.434 1.022 22.298 1.00 35.75 MOTA 910 ARG 0 1570 21.324 0.444 22.939 1.00 35.67 MOTA 911 GLU 1571 19.444 N 1.695 22.880 1.00 35.56 MOTA 913 CA GLU 1571 19.331 1.835 24.328 1.00 36.50 MOTA 914 CB GLU 1571 18.055 2.607 24.667 1.00 39.08 MOTA 915 CG GLU 1571 18.061 4.056 24.208 1.00 46.75

ATOM 916 CD GLU 1571 16.694 4.721 24.311 1.00 51.36 ATOM 917 OE1 GLU 1571 15.676 3.996 24.417 1.00 55.22 **ATOM** 918 OE2 GLU 1571 16.635 5.972 24.267 1.00 53.59 **ATOM** 919 C GLU 1571 19.314 0.469 25.022 1.00 34.82 **ATOM** 920 0 GLU 1571 20.018 0.242 26.013 1.00 35.05 MOTA 921 N TYR 1572 18.520 24.469 -0.441 1.00 33.35 MOTA 923 CA TYR 1572 -1.796 18.366 24.986 1.00 31.83 MOTA 924 CB TYR 1572 17.365 -2.544 24.102 1.00 30.77 ATOM 925 TYR CG 1572 17.170 -4.008 24.408 1.00 28.50 ATOM 926 CD1 TYR 1572 16.193 -4.420 25.313 1.00 30.48 **ATOM** 927 -5.760 CEI TYR 1572 15.977 25.574 1.00 30.97 **ATOM** 928 CD2 TYR 1572 17.933 -4.985 23.772 1.00 26.14 ATOM 929 CE2 TYR 1572 17.725 -6.329 24.027 1.00 26.21 MOTA 930 CZ TYR 1572 16.742 -6.708 24.935 1.00 .30.30 MOTA 931 OH TYR 1572 16.518 -8.041 25.214 1.00 33.52 MOTA 933 С TYR 1572 19.692 -2.556 25.044 1.00 34.83 MOTA 934 0 TYR 1572 19.959 -3.308 25.992 1.00 34.93 MOTA 935 N -2.370 LEU 1573 20.517 24.020 1.00 34.34 MOTA 937 CA LEU 1573 21.803 -3.053 23.961 1.00 35.38 MOTA 938 CB LEU 1573 22.357 -3.027 22.531 1.00 32.71 ATOM 939 CG LEU 1573 21.669 -3.891 21.464 1.00 29.16 ATOM 940 CD1 LEU 1573 22.161 -3.503 20.087 1.00 26.98 MOTA 941 CD2 LEU 1573 21.932 -5.351 21.710 1.00 28.85 MOTA 942 C LEU 1573 22.799 -2.420 24.933 1.00 37.54 MOTA 943 0 LEU 1573 23.511 -3.123 25.659 1.00 36.67 MOTA 944 N GLN 1574 22.814 -1.092 24.969 1.00 37.90 MOTA 946 CA GLN 1574 23.729 -0.368 25.838 1.00 39.77 MOTA 947 CB GLN 1574 23.624 1.138 25.572 1.00 40.09 MOTA 948 CG GLN 1574 24.208 1.549 24.217 1.00 42.28 ATOM 949 CD GLN 1574 24.030 3.018 23.896 1.00 44.28 MOTA 950 OE1 GLN 1574 23.362 3.755 24.615 1.00 47.55 MOTA 951 1574 NE2 GLN 24.613 3.448 22.790 1.00 46.09 MOTA 954 С GLN 1574 23.490 -0.697 27.310 1.00 40.75 MOTA 955 GLN 0 1574 24.440 -0.939 28.059 1.00 41.29 MOTA 956 N ALA 1575 22.220 -0.783 27.696 1.00 40.10 MOTA 958 CA ALA 1575 21.842 -1.088 29.069 1.00 38.81 MOTA 959 CB ALA 1575 20.349 -0.819 29.273 1.00 35.69 ATOM 960 ALA C 1575 22.192 -2.514 29.503 1.00 40.63 MOTA 961 O ALA 1575 22.098 -2.843 30.690 1.00 43.39 MOTA 962 N ARG 1576 22.602 -3.357 28.561 1.00 38.39 MOTA 964 CA ARG 1576 22.945 -4.729 28.896 1.00 37.69 MOTA 965 CB ARG 1576 22.034 -5.689 28.137 1.00 38.16 MOTA 966 CG ARG 1576 20.594 ~5.547 28.589 1.00 37.89 MOTA 967 CDARG 1576 19.622 -6.281 27.711 1.00 37.36 MOTA 968 NE ARG 1576 18.267 -6.255 28.265 1.00 34.99 MOTA 970 CZ ARG 1576 17.565 -5.150 28.484 1.00 36.94 ATOM 971 ARG NH1 1576 18.083 -3.960 28.209 1.00 36.1B **ATOM** 974 NH2 ARG 1576 16.310 -5.237 28.909 1.00 40.93 MOTA 977 C ARG 1576 24.413 -5.073 28.704 1.00 38.93 MOTA 978 O ARG 1576 24.801 -6.249 28.699 1.00 39.75 MOTA 979 N ARG 1577 25.233 -4.036 28.570 1.00 39.21 MOTA 981 CA ARG 1577 26.671 -4.196 28.413 1.00 38.97 ATOM 982 CB ARG 1577 27.307 -2.870 28.000 1.00 36.06 983 MOTA CG ARG 1577 26.992 -2.408 26.610 1.00 36.41

MOTA 984 CD ARG 1577 27.695 -1.094 26.337 1.00 36.17 MOTA 985 NE ARG 1577 27.776 -0.806 24.907 1.00 38.45 **ATOM** 987 czARG 1577 28.284 0.309 24.387 1.00 39.00 **ATOM** 988 NHI ARG 1577 28.764 1.262 25.175 1.00 38.88 ATOM 991 NH2 ARG 1577 28.311 0.469 23.071 1.00 37.76 **ATOM** 994 С ARG 1577 27.247 -4.571 29.772 1.00 40.59 **ATOM** 995 0 ARG 1577 26.680 -4.217 30.800 1.00 38.52 ATOM 996 N PRO 1578 28.358 -5.327 29.796 1.00 43.19 MOTA 997 CD PRO 1578 29.077 -5.980 28.692 1.00 44.84 MOTA 998 CA PRO 1578 28.952 -5.692 31.088 1.00 45.06 MOTA 999 CB PRO 1578 30.065 -6.673 30.689 1.00 44.86 MOTA 1000 CG PRO 1578 30.431 -6.229 29.308 1.00 44.56 MOTA 1001 С PRO 1578 29.513 -4.420 31.734 1.00 44.93 MOTA 1002 Ο, PRO - 1578 29.809 -3.439 31.043 1.00 43.13 1003 ATOM N PRO 1579 29.649 -4.414 33.067 1.00 47.61 MOTA 1004 CD PRO 1579 29.315 -5.492 34.012 1.00 48.39 MOTA 1005 CA PRO 1579 30.173 -3.247 33.784 1.00 48.74 MOTA 1006 CB PRO 1579 30.13B -3.706 35.238 1.00 49.73 MOTA 1007 CG PRO 1579 29.027 -4.711 35.259 1.00 49.21 MOTA 1008 C PRO 1579 31.591 -2.888 33.357 1.00 49.67 MOTA 1009 O PRO 1579 32.483 -3.733 33.361 1.00 52.07 MOTA 1010 N GLU 1592 19.165 -5.411 32.444 1.00 64.83 MOTA 1012 CA GLU 1592 20.603 -5.147 32.491 1.00 64.82 MOTA 1013 CB GLU 1592 20.969 -4.421 33.784 1.00 67.61 MOTA 1014 С GLU 1592 21.448 -6.413 32.335 1.00 63.99 MOTA 1015 0 GLU 1592 22.653 -6.336 32.098 1.00 65.67 MOTA 1016 N GLU 1593 20.821 -7.575 32.485 1.00 62.41 MOTA 1018 CA GLU 1593 21.534 -8.844 32.342 61.23 1.00 MOTA 1019 CB GLU 1593 20.595 -10.017 32.600 1.00 61.20 MOTA 1020 С GLU 1593 22.141 -8.953 30.944 1.00 59.26 MOTA 1021 0 GLU 1593 21.494 -8.631 29.945 1.00 59.84 MOTA 1022 N GLN 1594 23.388 -9.405 30.888 1.00 57.94 MOTA 1024 CA GLN 1594 24.101 -9.558 29.625 1.00 54.91 MOTA 1025 CB GLN 1594 25.501 -10.141 29.865 1.00 55.13 ATOM 1026 CG GLN 1594 26.439 -9.252 30.679 1.00 56.93 **ATOM** 1027 CD GLN 1594 27.682 -9.997 31.180 1.00 59.60 ATOM 1028 OE1 GLN 1594 28.241 -10.858 30.488 1.00 58.45 ATOM 1029 NE2 GLN 1594 28.117 -9.662 32.393 1.00 58.95 MOTA 1032 С GLN 1594 23.331 -10.43B 28.640 1.00 52.30 MOTA 1033 0 GLN 1594 22.637 -11.389 29.025 1.00 52.03 ATOM 1034 N LEU 1595 23.438 -10.091 27.366 1.00 49.60 MOTA 1036 CA LEU 1595 22.782 -10.836 26.308 1.00 45.16 ATOM 1037 CB LEU 1595 22.459 -9.907 25.135 1.00 41.36 MOTA 1038 CG LEU 1595 21.463 -8.815 25.523 1.00 39.43 MOTA 1039 CD1 LEU 1595 21.617 -7.583 24.644 1.00 36.21 MOTA 1040 CD2 LEU 1595 20.060 -9.389 25.480 1.00 34.91 MOTA 1041 C LEU 1595 23.747 -11.900 25.858 1.00 43.30 MOTA 1042 0 LEU 1595 24.953 -11.675 25.841 1.00 43.62 **ATOM** 1043 N SER 1596 23.230 -13.081 25.553 1.00 42.92 MOTA 1045 CA SER 1596 24.085 -14.150 25.077 1.00 41.86 MOTA 1046 CB SER 1596 23.410 -15.502 25.298 1.00 40.86 **ATOM** 1047 OG SER 1596 22.188 -15.596 24.595 1.00 37.88 MOTA 1049 C SER 1596 24.322 -13.914 23.587 1.00 41.59 **ATOM** 1050 0 SER 1596 23.657 -13.077 22.966 1.00 41.94

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ATOM 1051 N SER 1597 25.275 -14.637 23.018 1.00 39.60 MOTA 1053 CA SER 1597 25.557 -14.518 21.603 1.00 39.74 MOTA 1054 SER CB 1597 26.729 -15.409 21.223 1.00 41.38 **ATOM** 1055 OG SER 1597 27.824 -15.147 22.077 1.00 50.59 **ATOM** 1057 C SER 1597 24.315 -14.921 20.818 1.00 38.16 MOTA 1058 0 SER 1597 24.036 -14.353 19.769 1.00 38.03 ATOM 1059 N LYS 1598 23.560 -15.891 21.327 1.00 36.40 MOTA 1061 CA LYS 1598 22.362 -16.312 20.634 1.00 35.97 MOTA 1062 CB LYS 1598 21.791 -17.594 21.228 1.00 36.69 **ATOM** 1063 CG LYS 1598 20.989 -18.402 20.198 1.00 40.42 MOTA 1064 CD LYS 1598 20.164 -19.499 20.838 1.00 40.37 MOTA 1065 CE LYS 1598 19.792 -20.572 19.829 1.00 46.34 MOTA 1066 NZ · LYS 1598 20.993 -21.338 19.362 1.00 45.29 MOTA 1070 C LYS 1598 .. 21.324 ... -15.194 20.696 1.00 37.49 MOTA 1071 0 LYS 1598 20.567 -14.983 19.738 1.00 38.10 MOTA 1072 N ASP 1599 21.316 -14.458 21.807 1.00 35.21 MOTA 1074 CA ASP 1599 20.380 -13.352 21.983 1.00 34.02 MOTA 1075 CB ASP 1599 20.556 -12.686 23.346 1.00 37.78 MOTA 1076 CG ASP **159**9 19.970 -13.493 24.483 1.00 40.05 **ATOM** 1077 OD1 ASP 1599 20.270 -13.143 25.642 1.00 42.73 ATOM 1078 OD2 ASP 1599 19.204 -14.450 24.235 1.00 42.39 ATOM 1079 С ASP 1599 20.633 -12.306 20.922 1.00 32.84 MOTA 1080 O ASP 1599 19.694 -11.779 20.311 1.00 30.59 **ATOM** 1081 N LEU 1600 21.912 -11.999 20.724 1.00 31.11 **ATOM** 1083 CA LEU 1600 22.323 -10.998 19.744 1.00 32.17 **ATOM** 1084 CB LEU 1600 23.823 -10.722 19.875 1.00 32.30 MOTA 1085 CG LEU 1600 24.275 -10.162 21.235 1.00 31.08 1086 **MOTA** CD1 LEU 1600 25.794 -9.931 21.242 1.00 30.59 **ATOM** 1087 CD2 LEU 1600 23.549 -8.863 21.514 1.00 28.89 ATOM 1088 C LEU 1600 21.949 -11.390 18.311 1.00 30.77 MOTA 1089 0 LEU 1600 21.352 -10.601 17.574 1.00 29.87 ATOM 1090 N VAL 1601 22.269 -12.623 17.933 1.00 30.19 MOTA 1092 CA VAL 1601 21.954 -13.115 16.602 1.00 29.25 MOTA 1093 CB VAL 1601 22.593 -14.497 16.349 1.00 31.27 MOTA 1094 CG1 VAL 1601 22.355 -14.936 14.914 1.00 31.60 MOTA 1095 CG2 24.093 VAL 1601 -14.434 16.622 1.00 31.91 ATOM 1096 C VAL 1601 20.438 -13.181 16.405 1.00 29.06 ATOM 1097 -12.914 0 VAL 1601 19.946 15.310 1.00 27.71 MOTA 1098 N SER 1602 19.702 -13.511 17.468 1.00 29.10 ATOM 1100 CA SER 1602 18.243 -13.585 17.400 1.00 29.29 MOTA 1101 CB SER 1602 17.680 -14.189 18.679 1.00 30.B1 MOTA 1102 OG SER 1602 16.266 -14.074 18.692 1.00 35.78 ATOM 1104 С SER 1602 17.649 -12.199 17.156 1.00 28.98 ATOM 1105 0 SER 1602 16.662 -12.039 16.426 1.00 26.82 MOTA 1106 N CYS 1603 18.274 -11.202 17.765 1.00 29.06 ATOM 1108 CA CYS 1603 17.870 -9.823 17.599 1.00 29.22 ATOM -8.943 1109 CB CYS 1603 18.784 18.438 1.00 29.66 MOTA 1110 SG CYS 1603 18.575 -7.212 18.103 0.50 23.69 PRT1 MOTA 1111 C CYS 1603 17.988 -9.422 16.112 1.00 29.23 MOTA 1112 0 CYS 1603 17.087 -8.796 15.552 1.00 27.52 MOTA 1113 N ALA 1604 19.113 -9.778 15.491 1.00 27.87 MOTA 1115 CA ALA 1604 19.376 -9.484 14.077 1.00 26.37 MOTA 1116 CB ALA 1604 20.783 -9.941 13.690 1.00 23.88 MOTA 1117 С ALA 1604 18.349 -10.203 13.223 1.00 25.82

MOTA 1118 0 ALA 1604 17.788 -9.631 12.289 1.00 25.84 **MOTA** 1119 N TYR 1605 18.119 -11.468 13.544 1.00 25.56 **ATOM** 1121 CA TYR 1605 17.152 -12.276 12.827 1.00 27.81 MOTA 1122 CB TYR 1605 17.080 -13.662 13.456 1.00 26.66 MOTA 1123 CG TYR 1605 15.974 -14.515 12.886 1.00 30.75 **MOTA** 1124 CD1 TYR 1605 16.111 -15.141 11.640 1.00 30.20 MOTA 1125 CE1 TYR 1605 15.088 -15.944 11.126 1.00 30.03 MOTA 1126 CD2 TYR 1605 14.790 -14.707 13.596 1.00 30.73 **ATOM** 1127 CE2 TYR 1605 13.775 -15.500 13.097 1.00 30.71 MOTA 1128 CZTYR 1605 13.930 -16.117 11.867 1.00 30.93 MOTA 1129 OH TYR 1605 12.923 -16.928 11.417 1.00 32.31 MOTA 1131 С TYR 1605 15.748 -11.641 12.775 1.00 26.15 MOTA 1132 0 TYR 1605 15.147 -11.551 11.702 1.00 26.64 ATOM 1133 N GLN 1606 15.244 -11.200 13.926-1.00 25.48 MOTA 1135 CA GLN 1606 13.921 -10.581 14.023 1.00 26.86 MOTA 1136 CB **GLN** 1606 13.589 -10.269 15.482 1.00 26.83 ATOM 1137 CG GLN 1606 13.357 -11.508 16.332 1.00 25.84 MOTA 1138 CD GLN 1606 13.151 -11.167 17.791 1.00 30.86 **ATOM** 1139 OE1 **GLN** 1606 12.202 -10.471 18.150 1.00 31.87 **ATOM** 1140 NE2 GLN 1606 14.056 -11.631 18.640 1.00 31.67 MOTA 1143 С GLN 1606 13.835 -9.310 13.186 1.00 27.52 ATOM 1144 0 GLN 1606 12.831 -9.058 12.506 1.00 26.05 ATOM 1145 14.904 N VAL 1607 -8.523 13.216 1.00 26.68 MOTA 1147 CA VAL 1607 -7.301 14.963 12.435 1.00 25.66 MOTA 1148 CB VAL 1607 16.225 -6.485 12.787 1.00 28.50 MOTA 1149 CG1 VAL 1607 16.363 -5.274 11.853 1.00 26.04 MOTA 1150 CG2 VAL 1607 16.151 -6.031 14.246 1.00 24.45 MOTA 1151 С VAL 1607 14.934 -7.641 10.938 1.00 24.89 MOTA 1152 0 VAL 1607 14.184 -7.033 10.177 1.00 25.86 MOTA 1153 N ALA 1608 15.738 -8.619 10.522 1.00 25.24 MOTA 1155 CA -9.039 ALA 1608 15.773 9.120 1.00 22.95 MOTA 1156 CB ALA 1608 -10.117 16.813 8.920 1.00 20.24 MOTA 1157 C ALA 1608 14.383 -9.541 8.679 1.00 25.71 MOTA 1158 O ALA 1608 13.963 -9.319 7.532 1.00 27.48 MOTA 1159 N ARG 1609 13.676 -10.216 9.585 1.00 27.10 MOTA 1161 CA ARG 1609 12.327 -10.708 9.301 1.00 28.55 MOTA 1162 CB ARG 1609 11.840 -11.640 10.397 1.00 31.53 MOTA 1163 CG ARG 1609 12.407 -13.005 10.290 1.00 36.05 MOTA 1164 CD ARG 1609 11.537 -13.931 11.056 1.00 40.28 MOTA 1165 NE ARG 1609 10.849 -14.874 10.190 1.00 42.06 MOTA 1167 CZ ARG 1609 9.974 -15.771 10.632 1.00 42.08 MOTA 1168 NH1 ARG 9.678 1609 -15.834 11.928 1.00 40.32 MOTA 1171 NH2 ARG 1609 9.416 -16.620 9.784 1.00 43.27 MOTA 1174 С ARG 1609 11.329 -9.569 9.124 1.00 25.55 MOTA 1175 0 ARG 1609 -9.621 10.469 8.231 1.00 26.98 MOTA 1176 N GLY 1610 11.418 9.996 -8.565 1.00 23.92 MOTA 1178 CA GLY 1610 10.555 -7.406 9.870 1.00 22.19 MOTA 1179 C 1610 GLY 10.800 -6.747 8.512 1.00 25.92 MOTA 1180 0 GLY 1610 9.855 -6.424 7.772 1.00 23.49 MOTA 1181 N MET -6.589 1611 12.076 8.163 1.00 23.15 MOTA 1183 CA MET 1611 12.456 -5.989 6.888 1.00 22.57 MOTA 1184 CB MET 1611 13.956 -5.710 6.849 1.00 22.18 MOTA 1185 CG MET 1611 14.398 -4.542 7.729 1.00 22.63 MOTA 1186 SD MET 1611 13.478 -3.006 7.426 1.00 25.23

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ATOM 1187 CE MET 1611 13.812 -2.688 5.675 1.00 21.38 MOTA 1188 1611 12.050 C MET -6.848 5.681 1.00 23.96 MOTA 1189 0 MET 1611 11.673 -6.326 4.633 1.00 25.26 MOTA 1190 N GLU 1612 12.130 -8.163 5.822 1.00 24.34 11.755 MOTA 1192 CA GLU 1612 -9.043 4.733 1.00 25.56 **ATOM** 1193 CB GLU 1612 12.018 -10.494 5.121 1.00 24.96 MOTA 1194 CG GLU 1612 11.703 -11.488 4.009 1.00 26.79 **ATOM** 1195 CDGLU 1612 11.812 -12.931 4.450 1.00 26.96 ATOM 1196 11.557 OE1 GLU 1612 -13.212 5.636 1.00 30.98 MOTA 1197 OE2 GLU 1612 12.154 -13.791 3.611 1.00 32.31 ATOM С 1198 GLU 1612 10.267 -8.829 4.415 1.00 25.70 MOTA 1199 О GLU 1612 9.860 -8.753 3.252 1.00 24.30 MOTA 1200 N TYR 1613 9.463 · -8.723 5.465 1.00 23.55 ATOM. __1202 __.CA TYR 1613 8.037 -8.501 5.294 1.00 -22.94 --1203 MOTA CB TYR 1613 7.314 -8.586 6.650 1.00 24.00 MOTA 1204 CG TYR 1613 5.841 -8.281 6.549 1.00 22.93 MOTA 1205 CD1 TYR 1613 4.945 -9.245 6.097 1.00 21.60 MOTA 1206 CE1 TYR 1613 3.582 -8.962 5.963 1.00 21.14 MOTA 1207 CD2 TYR 1613 5.347 -7.018 6.869 1.00 25.81 MOTA 1208 CE2 TYR 1613 3.979 -6.718 6.733 1.00 24.45 **ATOM** 1209 CZTYR 1613 3.112 -7.697 6.281 1.00 23.28 MOTA 1210 OH TYR 1613 1.775 -7.411 6.126 1.00 22.95 ATOM 1212 С TYR 1613 7.803 -7.138 4.637 1.00 22.57 MOTA 1213 0 TYR 1613 7.022 -7.024 3.699 1.00 24.72 MOTA 1214 N LEU 1614 8.460 -6.101 5.156 1.00 22.16 MOTA 1216 CA LEU 1614 8.334 -4.755 4.615 1.00 22.60 MOTA 1217 CB 9.175 -3.772 LEU 1614 5.440 1.00 22.56 MOTA 1218 CG LEU 1614 8.577 -3.415 6.802 1.00 24.92 MOTA 1219 CD1 LEU 1614 9.535 -2.541 7.580 1.00 21.46 MOTA 1220 CD2 LEU 1614 7.218 -2.711 6.611 1.00 21.87 MOTA 1221 C LEU 1614 8.699 -4.683 3.124 1.00 23.76 MOTA 1222 0 LEU 1614 7.975 -4.077 2.326 1.00 23.84 MOTA 1223 N ALA 1615 9.809 -5.314 2.744 1.00 23.48 MOTA 1225 CA ALA 1615 10.232 -5.340 1.352 1.00 22.70 ATOM 1226 CB ALA 1615 11.591 -6.019 1.215 1.00 21.52 MOTA 1227 С ALA 1615 9.188 -6.063 0.505 1.00 22.87 MOTA 1228 O ALA 1615 8.854 -5.591 -0.581 1.00 24.23 MOTA 1229 N SER 1616 8.652 -7.176 1.015 1.00 22.76 ATOM 1231 CA SER 1616 7.638 -7.954 0.295 1.00 22.88 ATOM 1232 CB SER 1616 7.315 -9.251 1.039 1.00 21.39 MOTA 1233 OG SER 1616 6.400 -9.036 .2.102 1.00 26.24 MOTA 1235 C SER 1616 6.360 -7.131 0.044 1.00 24.88 MOTA 1236 0 1616 SER 5.635 -7.358 -0.927 1.00 24.73 MOTA 1237 N LYS 1617 6.104 -6.173 0.927 1.00 23.82 MOTA 1239 CA LYS 1617 4.970 -5.287 0.810 1.00 22.47 MOTA 1240 CB LYS 1617 4.455 -4.914 2.199 1.00 23.62 MOTA 1241 CG LYS 1617 3.792 -6.072 2.927 1.00 27.16 MOTA 1242 CD LYS 1617 2.551 -6.487 2.169 1.00 30.84 MOTA 1243 CE LYS 1617 1.810 -7.602 2.852 1.00 33.57 **ATOM** 1244 NZ LYS 1617 2.484 -8.894 2.653 1.00 44.30 MOTA 1248 С LYS 1617 5.346 -4.034 0.035 1.00 23.56 MOTA 1249 0 LYS 1617 4.639 -3.030 0.091 1.00 25.16 ATOM 1250 N LYS 1618 6.495 -4.066 -0.638 1.00 24.69 MOTA 1252 CA LYS 1618 6.953 -2.943 -1.468 1.00 24.04

ATOM 1253 CB 5.863 LYS 1618 -2.581 -2.492 1.00 26.96 **ATOM** 1254 CG LYS 1618 5.775 -3.491 -3.709 1.00 29.14 ATOM 1255 CD LYS 1618 5.567 -4.942 -3.345 1.00 33.91 ATOM 1256 CE LYS 1618 5.662 -5.858 -4.558 1.00 32.98 **ATOM** 1257 NZ LYS 1618 4.431 -5.380 -5.821 1.00 36.73 MOTA 1261 С LYS 1618 7.406 -1.686 -0.713 1.00 24.01 MOTA 1262 0 LYS 1618 7.557 -0.606 -1.302 1.00 23.73 MOTA 1263 N CYS 1619 7.689 -1.842 0.573 1.00 25.91 MOTA 1265 CA CYS 1619 8.108 -0.731 1.418 1.00 25.65 MOTA 1266 CB CYS 1619 7.444 -0.885 2.792 1.00 24.93 **ATOM** 1267 SG CYS 1619 7.941 0.313 4.064 1.00 28.14 MOTA 1268 C CYS 1619 9.631 -0.628 1.573 1.00 23.07 MOTA 1269 0 CYS 1619 10.304 -1.630 1.809 1.00 20.98 22.95 MOTA 1270 N ---- ILE 1620 10.170 0.573 1.363 1.00 MOTA 1272 CA ILE 1620 11.604 0.841 1.524 1.00 23.81 **ATOM** 1273 CB ILE 1620 12.202 1.607 0.276 1.00 24.36 MOTA 1274 CG2 ILE 1620 13.670 1.995 0.506 1.00 17.24 MOTA 1275 CG1 ILE 1620 12.108 0.739 -0.987 1.00 23.13 MOTA 1276 CD1 ILE 1620 12.171 1.544 -2.286 1.00 25.37 MOTA 1277 С ILE 1620 11.633 1.729 2.771 1.00 24.70 MOTA 1278 0 ILE 1620 10.981 2.763 2.806 1.00 25.21 MOTA 1279 N HIS 1621 12.348 1.297 3.804 1.00 25.62 MOTA 1281 CA HIS 1621 12.427 2.041 5.057 1.00 25.53 MOTA 1282 CB HIS 1621 13.181 1.237 6.132 1.00 22.76 MOTA 1283 CG HIS 1621 13.004 1.773 7.528 1.00 26.42 MOTA 1284 CD2 HIS 1621 12.356 1.260 8.601 1.00 24.74 MOTA 1285 ND1 HIS 1621 13.474 3.011 7.927 1.00 26.62 MOTA 1287 CE1 HIS 1621 13.119 3.233 9.179 1.00 25.70 ATOM 1288 NE2 HIS 1621 12.439 2.187 9.616 1.00 26.23 MOTA 1290 C HIS 1621 13.073 3.401 4.914 1.00 26.36 MOTA 1291 0 HIS 1621 12.528 4.405 5.370 1.00 25.89 MOTA 1292 N ARG 1622 14.271 3.406 4.341 1.00 25.35 MOTA 1294 CA ARG 1622 15.082 4.608 4.140 1.00 25.05 MOTA 1295 CB ARG 1622 14.268 5.766 3.540 1.00 20.89 MOTA 1296 CG ARG 1622 13.709 5.444 2.175 1.00 19.03 MOTA 1297 CD ARG 1622 13.089 6.656 1.488 0.50 14.06 MOTA 1298 NE ARG 1622 12.684 6.300 0.131 0.50 11.96 MOTA 1300 CZ ARG 1622 11.606 5.577 -0.166 0.50 11.83 MOTA 1301 NH1 ARG 1622 10.801 5.137 0.797 0.50 10.20 MOTA 1304 NH2 ARG 1622 -1.425 11.366 5.239 0.50 8.63 **ATOM** 1307 С ARG 1622 15.877 5.058 5.379 1.00 24.37 MOTA 1308 0 ARG 1622 16.787 5.863 5.268 1.00 25.17 MOTA 1309 ASP N 1623 15.555 4.527 6.552 1.00 24.61 ATOM 1311 CA ASP 1623 16.315 4.899 7.748 1.00 28.82 MOTA 1312 CB ASP 1623 15.777 6.173 8.410 1.00 32.33 ATOM 1313 CG ASP 1623 16.733 6.735 9.469 1.00 36.67 MOTA 1314 OD1 **ASP** 1623 16.276 7.520 10.321 1.00 43.56 ATOM 1315 OD2 ASP 1623 17.937 6.385 9.463 1.00 36.29 **ATOM** 1316 C ASP 1623 16.408 3.766 8.766 1.00 28.22 **ATOM** 1317 0 ASP 1623 16.118 3.937 9.956 1.00 26.87 MOTA 1318 N LEU 1624 16.783 2.592 8.278 1.00 26.34 MOTA 1320 CA LEU 1624 16.941 1.428 9.132 1.00 26.59 MOTA 1321 CB LEU 1624 16.996 0.168 8.265 1.00 24.59 **ATOM** 1322 CG LEU 1624 17.082 -1.175 8.978 1.00 24.72

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ATOM 1323 CD1 LEU 1624 15.844 -1.408 9.856 1.00 24.35 **ATOM** 1324 CD2 LEU 1624 17.258 -2.261 7.931 1.00 24.63 ATOM 1325 C LEU 1624 18.210 1.595 10.004 1.00 26.87 **ATOM** 1326 0 LEU 1624 19.322 1.777 9.497 1.00 28.19 **ATOM** 1327 N ALA 1625 18.009 1.570 11.317 1.00 27.77 MOTA 1329 CA ALA 1625 19.069 1.741 12.309 1.00 24.54 **ATOM** 1330 CB ALA 1625 19.355 3.210 12.494 1.00 19.81 **ATOM** 1331 C ALA 1625 18.498 1.173 13.592 1.00 26.44 MOTA 1332 O ALA 1625 17.289 0.961 13.679 1.00 27.58 MOTA 1333 N ALA 1626 19.342 0.940 14.594 1.00 25.38 MOTA 1335 CA ALA 1626 18.872 0.397 15.865 1.00 24.65 MOTA 1336 CB ALA 1626 20.054 0.023 16.774 1.00 23.35 ATOM 1337 C ALA 1626 17.929 1.373 16.578 1.00 25.54 MOTA 1338 0 ALA 1626 __ 17..057 0.951 27.70 17.325 1.00 1339 MOTA N ARG 1627 18.104 2.671 16.344 1.00 25.06 1341 MOTA CA ARG 1627 17.242 3.675 16.959 1.00 25.48 MOTA 1342 CB ARG 1627 17.706 5.089 16.597 1.00 28.15 MOTA 1343 CG ARG 1627 17.759 5.370 15.084 1.00 33.13 MOTA 1344 CD ARG 1627 18.157 6.811 14.774 1.00 33.29 MOTA 1345 NF. ARG 1627 18.442 7.011 13.351 1.00 35.74 MOTA 1347 CZ ARG 1627 19.652 6.889 12.813 1.00 37.40 MOTA 1348 NH1 ARG 1627 20.695 6.585 13.575 1.00 39.73 MOTA 1351 NH2 ARG 1627 19.817 7.012 11.507 1.00 36.90 MOTA 1354 С ARG 1627 15.812 3.491 16.479 1.00 24.81 ATOM 1355 0 ARG 1627 14.871 3.853 17.173 1.00 24.05 MOTA 1356 N ASN 1628 15.667 2.910 15.293 1.00 24.80 MOTA 1358 CA ASN 1628 14.368 2.686 14.685 1.00 25.97 MOTA 1359 CB ASN 1628 14.383 3.132 13.225 1.00 30.08 MOTA 1360 CG ASN 1628 14.417 4.640 13.096 1.00 33.62 MOTA 1361 OD1 ASN 1628 13.775 5.347 13.864 1.00 35.11 MOTA 1362 ND2 ASN 1628 15.212 5.141 12.169 1.00 36.31 **ATOM** 1365 C ASN 1628 13.802 1.288 14.824 1.00 26.03 MOTA 1366 0 ASN 1628 12.951 0.869 14.031 1.00 26.87 MOTA 1367 N VAL 1629 14.330 0.550 15.797 1.00 26.04 MOTA 1369 CA VAL 1629 13.854 -0.783 16.128 1.00 25.09 MOTA 1370 CB VAL 1629 14.924 -1.876 15.959 1.00 27.00 MOTA 1371 CG1 VAL 1629 14.390 -3.197 16.546 1.00 20.99 MOTA 1372 CG2 VAL 1629 15.295 -2.051 14.462 1.00 23.26 MOTA 1373 C VAL 1629 13.504 -0.671 17.600 1.00 27.59 MOTA 1374 0 VAL 1629 14.340 -0.285 18.418 1.00 25.81 MOTA 1375 N LEU 1630 12.245 -0.929 17.923 1.00 28.17 MOTA 1377 CA LEU 1630 11.768 -0.845 19.296 1.00 30.20 MOTA 1378 CB LEU 1630 10.445 -0.077 19.332 1.00 30.26 ATOM 1379 CG LEU 1630 10.484 1.285 18.626 1.00 29.81 MOTA 1380 CD1 LEU 1630 9.119 1.983 18.745 1.00 28.46 MOTA 1381 CD2 LEU 1630 11.576 2.141 19.233 1.00 28.37 MOTA 1382 С LEU 1630 11.639 -2.242 19.904 1.00 29.32 ATOM 1383 0 LEU 1630 11.414 -3.219 1.00 19.189 30.84 MOTA 1384 N VAL 1631 11.800 -2.342 21.221 1.00 28.90 MOTA 1386 CA VAL 1631 11.732 -3.629 21.905 1.00 26.84 MOTA 1387 CB VAL 1631 13.067 -3.919 22.670 1.00 28.88 **ATOM** 1388 CG1 VAL 1631 13.077 -5.341 23.236 1.00 21.54 MOTA 1389 CG2 VAL 1631 14.259 -3.699 21.744 1.00 24.30 MOTA 1390 С VAL 1631 10.561 -3.645 22.881 1.00 29.02

MOTA	1391	0	VAL	1631	10.406	-2.737	23.706	1.00	29.31
MOTA	1392	N	THR	1632	9.733	-4.674	22.764	1.00	30.84
MOTA	1394	CA	THR	1632	8.562	~4.830	23.616	1.00	32.24
MOTA	1395	CB	THR	1632	7.488	-5.685	22.912	1.00	31.45
ATOM	1396	OG1	THR	1632	7.896	-7.064	22.910	1.00	30.86
ATOM	1398	CG2	THR	1632	7.268	-5.194	21.470	1.00	28.04
MOTA	1399	C	THR	1632	8.919	-5.493	24.943	1.00	34.17
ATOM	1400	0	THR	1632	10.017	-6.019	25.105	1.00	35.02
MOTA	1401	N	GLU	1633	7.959	-5.524	25.866	1.00	36.16
MOTA	1403	CA	GLU	1633	8.155	-6.138	27.177	1.00	36.34
MOTA	1404	CB	GLU	1633	6.865	-6.063	27.996	1.00	37.07
ATOM	1405	CG	GLU	1633	6.957	-6.649	29.414	1.00	44.57
MOTA	1406	CD	' GLU	1633	8.035	-6.000	30.301	1.00	49.38
ATOM	1407	OE1	GLU	1633	8.124	-4:753	30.352	1.00	51.03
ATOM	1408	OE2	GLU	1633	8.788	-6.750	30.968	1.00	51.63
ATOM	1409	С	GLU	1633	8.600	-7.585	27.042	1.00	36.42
MOTA	1410	0	GLU	1633	9.347	-8.085	27.874	1.00	38.56
MOTA	1411	N	ASP	1634	8.185	-8.240	25.964	1.00	37.70
ATOM	1413	CA	ASP	1634	8.550	-9.637	25.737	1.00	38.53
ATOM	1414	CB	ASP	1634	7.408	-10.378	25.027	1.00	44.08
ATOM	1415	CG	ASP	1634	6.041	-10.106	25.657	1.00	51.60
ATOM	1416	OD1	ASP	1634	5.865	-10.367	26.867	1.00	52.37
MOTA	1417	OD2	ASP	1634	5.137	-9.631	24.933	1.00	57.23
MOTA	1418	С	ASP	1634	9.826	-9.776	24.905	1.00	36.56
MOTA	1419	0	ASP	1634	10.127	-10.865	24.430	1.00	36.74
ATOM	1420	N	ASN	1635	10.569	-8.683	24.739	1.00	36.56
MOTA	1422	CA	ASN	1635	11.819	-8.662	23.945	1.00	37.10
MOTA	1423	CB	ASN	1635	12.888	-9.587	24.548	1.00	36.92
ATOM	1424	CG	ASN	1635	13.226	-9.226	25.978	1.00	36.54
MOTA	1425	OD1	ASN	1635	13.275	-8.058	26.340	1.00	38.84
MOTA	1426	ND2	ASN	1635	13.423	-10.235	26.806	1.00	39.58
ATOM	1429	С	ASN	1635	11.632	-8.980	22.451	1.00	34.78
MOTA	1430	0	ASN	1635	12.446	-9.677	21.834	1.00	34.00
MOTA	1431	N	VAL	1636	10.533	-8.498	21.880	1.00	31.35
MOTA	1433	CA	VAL	1636	10.279	-8.711	20.469	1.00	29.76
ATOM	1434	CB	VAL	1636	8.778	-8.946	20.181	1.00	30.60
ATOM	1435	CG1	VAL	1636	8.538	-9.081	18.675	1.00	30.38
ATOM	1436	CG2	VAL	1636	8.315	-10.209	20.897	1.00	28.51
MOTA	1437	С	VAL	1636	10.768	-7.449	19.781	1.00	28.02
MOTA	1438	0	VAL	1636	10.506	-6.351	20.254	1.00	25.87
MOTA	1439	N	MET	1637	11.575	-7.624	18.738	1.00	28.15
MOTA	1441	CA	MET	1637	12.119	-6.508	17.980	1.00	26.01
ATOM	1442	CB	MET	1637	13.366	-6.953	17.204	1.00	27.82
ATOM	1443	CG	MET	1637	14.479	-7.554	18.051	1.00	29.73
MOTA	1444	SD	MET	1637	15.124	-6.410	19.288	1.00	29.96
MOTA	1445	CE	MET	1637	15.120	-7.459	20.689	1.00	27.19
MOTA	1446	С	MET	1637	11.040	-6.087	16.993	1.00	24.77
MOTA	1447	0	MET	1637	10.480	-6.929	16.303	1.00	24.50
MOTA	1448	N	LYS	1638	10.755	-4.791	16.931	1.00	25.74
MOTA	1450	CA	LYS	1638	9.746	-4.258	16.029	1.00	23.67
MOTA	1451	CB	LYS	1638	8.486	-3.888	16.799	1.00	21.78
MOTA	1452	CG	LYS	1638	7.715	-5.092	17.298	1.00	24.60
MOTA	1453	CD	LYS	1638	6.406	-4.683	18.005	1.00	23.87
MOTA	1454	CE	LYS	1638	5.486	-5.897	18.256	1.00	23.06

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ATOM 1455 NZ LYS 1638 4.871 -6.398 16.976 1.00 24.60 MOTA 1459 1638 С LYS 10.260 -3.042 15.293 1.00 24.37 MOTA 1460 0 LYS 1638 10.658 -2.055 15.901 1.00 26.58 MOTA 1461 N ILE 1639 10.271 -3.119 13.971 1.00 25.69 MOTA 1463 CA ILE 1639 10.721 -2.005 13.148 1.00 25.94 **ATOM** 1464 CB ILE 1639 10.935 -2.447 11.668 1.00 26.49 ATOM 1465 CG2 ILE 1639 11.218 -1.236 10.762 1.00 21.19 ATOM CG1 1466 ILE 1639 12.103 -3.433 11.604 1.00 27.58 MOTA 1467 CD1 ILE 1639 12.120 -4.232 10.355 1.00 32.96 MOTA 1468 C ILE 1639 9.675 -0.892 13.242 1.00 27.32 MOTA 1469 0 ILE 1639 8.466 -1.133 13.103 1.00 25.45 MOTA 1470 N ALA 1640 10.156 0.320 13.498 1.00 27.43 MOTA 1472 CA ALA 1640 9.321 1.499 13.632 1.00 26.96 MOTA 1473 СВ ALA 1640 9.557 2.133 15.006 1.00 25.21 MOTA 1474 C ALA 1640 1.00 9.641 2.510 12.538 26.80 **ATOM** 1475 0 ALA 1640 10.691 2.446 11.896 1.00 27.55 **ATOM** 1476 N ASP 1641 8.716 3.440 12.328 1.00 27.06 **ATOM** 1478 CA **ASP** 1641 8.862 4.526 11.349 1.00 30.54 **ATOM** 1479 CB ASP 1641 9.993 5.484 11.753 1.00 33.12 **ATOM** 1480 CG 1641 ASP 9.668 6.310 12.999 1.00 36.17 MOTA 1481 OD1 ASP 1641 10.477 7.203 13.334 1.00 42.24 MOTA 1482 OĎ2 ASP 1641 8.633 6.076 13.648 1.00 33.22 MOTA 1483 C ASP 1641 9.049 4.107 9.898 1.00 29.94 MOTA 1484 0 **ASP** 1641 1.00 9.598 4.861 9.102 30.13 ATOM 1485 N PHE 1642 8.569 2.920 9.553 1.00 30.22 ATOM 1487 CA PHE 1642 8.680 2.426 8.191 1.00 30.91 **ATOM** 1488 CB PHE 1642 8.462 0.909 8.159 1.00 26.24 ATOM 1489 CG PHE 1642 7.156 0.470 8.750 1.00 27.82 **ATOM** 1490 CD1 PHE 1642 5.986 0.495 7.988 1.00 27.08 MOTA 1491 CD2 PHE 1642 7.089 0.026 10.066 1.00 26.70 1492 **ATOM** CE1 PHE 1642 4.761 0.088 8.532 1.00 25.18 ATOM 1493 CE2 ~0.383 PHE 1642 5.872 10.624 1.00 27.59 **ATOM** 1494 CZPHE 1642 4.705 ~0.354 9.855 1.00 28.05 MOTA 1495 C PHE 1642 7.729 3.139 7.219 1.00 33.35 MOTA 1496 0 PHE 1642 7.983 3.165 6.01B 1.00 36.19 MOTA 1497 N GLY 1643 6.661 3.746 7.736 1.00 32.76 MOTA 1499 CA GLY 1643 5.710 4.419 6.863 1.00 31.44 MOTA 1500 C GLY 1643 5.805 6.910 5.927 1.00 32.94 MOTA 1501 0 GLY 1643 4.945 6.636 6.399 1.00 33.10 MOTA 1502 N LEU 1644 6.872 6.407 7.525 1.00 35.45 MOTA 1504 CA LEU 1644 7.124 7.828 7.684 1.00 39.04 MOTA 1505 CB LEU 1644 8.387 8.011 8.514 1.00 37.80 MOTA 1506 CG LEU 1644 8.414 9.120 9.549 1.00 42.51 ATOM 1507 CD1 LEU 1644 7.301 8.887 10.563 1.00 44.08 ATOM 1508 CD2 LEU 1644 9.779 9.127 10.243 1.00 44.47 MOTA 1509 C LEU 1644 7.259 8.580 6.357 1.00 42.20 MOTA 1510 0 LEU 1644 7.895 8.107 5.414 1.00 44.14 MOTA 1511 N ALA 1645 6.607 9.732 6.267 1.00 43.89 MOTA 1513 CA ALA 1645 6.677 10.569 5.082 1.00 45.62 MOTA 1514 CB ALA 1645 5.463 11.493 5.028 1.00 45.06 **ATOM** 1515 С ALA 1645 7.966 11.388 5.186 1.00 45.82 MOTA 1516 0 ALA 1645 8.240 11.994 6.228 1.00 45.85 MOTA 1517 N ARG 1646 8.766 11.389 4.129 1.00 45.16 MOTA 1519 CA ARG 1646 10.015 12.140 4.138 1.00 47.06

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ATOM 1520 CB ARG 1646 11.126 11.318 4.794 1.00 48.00 **ATOM** 1521 С ARG 1646 10.445 12.546 2.742 1.00 46.83 ATOM 1522 0 ARG 1646 10.429 11.729 1.823 1.00 45.76 **ATOM** 1523 N ASP 1647 10.807 13.814 2.578 1.00 48.96 MOTA 1525 CA ASP 1647 11.278 14.291 1.288 1.00 50.93 MOTA 1526 CB **ASP** 1647 10.938 15.769 1.073 1.00 52.33 1527 MOTA CG **ASP** 1647 11.191 16.228 -0.360 1.00 55.93 MOTA 1528 OD1 **ASP** 1647 12.231 15.850 -0.956 1.00 52.58 MOTA 1529 OD2 **ASP** 1647 10.340 16.980 -0.896 1.00 59.54 **ATOM** 1530 C ASP 1647 12.789 14.104 1.336 1.00 50.78 ATOM 1531 ASP 1647 O 13.491 14.803 2.077 1.00 48.32 MOTA 1532 N ILE 1648 13.274 13.144 0.556 1.00 50.84 MOTA 1534 CA ILE 1648 14.696 12.833 0.516 1.00 52.58 ATOM -1535 CB ILE 1648 14.984 11.571 1.00 -50.85 ----0.324 MOTA 1536 CG2 ILE 1648 14.204 10.386 0.241 1.00 49.34 MOTA 1537 CG1 ILE 1648 14.638 11.813 -1.801 1.00 48.22 MOTA 1538 CD1 ILE 1648 15.233 10.806 -2.754 1.00 42.86 **ATOM** 1539 С ILE 1648 15.523 13.999 -0.018 1.00 55.57 MOTA 1540 0 ILE 1648 16.648 14.222 0.423 1.00 57.24 **ATOM** 1541 N HIS 1649 14.944 14.766 -0.936 1.00 56.80 MOTA 1543 CA HIS 1649 15.650 15.895 -1.520 1.00 58.03 MOTA 1544 CB HIS 1649 15.013 16.302 -2.859 1.00 58.71 MOTA 1545 CG HIS 1649 -3.958 15.221 15.308 1.00 60.28 MOTA 1649 1546 CD2 HIS 16.303 14.566 -4.306 1.00 60.74 MOTA 1547 ND1 HIS 1649 14.241 14.986 -4.874 1.00 61.70 MOTA 1549 CE1 HIS 1649 14.708 14.104 -5.742 1.00 61.86 MOTA 1550 NE2 HIS 1649 15.959 13.833 -5.417 1.00 60.98 MOTA 1552 C HIS 1649 15.721 17.093 -0.591 1.00 58.49 MOTA 1553 0 HIS 1649 16.129 18.175 -1.004 1.00 60.56 ATOM 1554 HIS N 1650 15.285 16.916 0.654 1.00 59.58 **MOTA** 1556 CA HIS 1650 15.306 18.001 1.635 1.00 61.38 **ATOM** 1557 CB HIS 1650 13.898 18.540 1.863 1.00 65.28 **ATOM** 1558 CG HIS 1650 13.404 19.433 0.738 1.00 72.62 ATOM 1559 CD2 HIS 1650 13.492 20.752 0.536 1.00 76.23 MOTA 1560 ND1 HIS 1650 12.710 18.904 -0.339 1.00 77.05 MOTA 1562 CEl HIS 1650 12.402 19.907 -1.157 1.00 78.51 MOTA 1563 NE2 HIS 1650 12.863 21.015 -0.647 1.00 78.82 MOTA 1565 C HIS 1650 15.925 17.575 2.972 1.00 60.63 MOTA 1566 0 HIS 1650 15.796 18.271 3.969 1.00 60.20 MOTA 1567 16.584 N ILE 1651 16.419 2.987 1.00 60.22 **ATOM** 1651 1569 CA ILE 17.197 15.920 4.204 1.00 60.03 **ATOM** 1570 CB ILE 1651 17.574 14.434 4.069 1.00 62.54 MOTA 1571 CG2 ILE 1651 18.280 13.920 5.323 1.00 63.48 ATOM 1572 CG1 ILE 1651 16.329 13.584 3.800 1.00 65.18 **ATOM** 1573 CD1 ILE 1651 16.635 12.124 3.603 1.00 67.18 **ATOM** 1574 C ILE 1651 18.457 16.698 4.557 1.00 59.16 MOTA 1575 0 ILE 1651 19.326 16.907 3.716 1.00 59.25 MOTA 1576 ASP N 1652 18.532 17.176 5.793 1.00 58.91 MOTA 1578 CA ASP 1652 19.702 17.915 6.260 1.00 58.25 MOTA 1579 CB ASP 1652 19.312 18.788 7.444 1.00 61.14 **ATOM** 1580 CG ASP 1652 20.506 19.569 8.028 1.00 65.33 MOTA 1581 OD1 ASP 1652 21.614 19.574 7.411 1.00 67.11 **ATOM** 1582 OD2 ASP 1652 20.337 20.191 9.126 1.00 69.04 ATOM 1583 C ASP 1652 20.786 16.922 6.676 1.00 56.75

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ATOM 1584 0 ASP 1652 20.699 16.307 7.741 1.00 56.06 MOTA 1585 N TYR 1653 21.794 16.762 5.826 1.00 55.40 **ATOM** 1587 CA TYR 1653 22.900 15.849 6.088 1.00 54.50 MOTA 1588 CB 1653 23.825 TYR 15.783 4.872 1.00 52.80 **ATOM** 1589 CG TYR 1653 23.334 14.854 3.796 1.00 52.10 **ATOM** 1590 CD1 TYR 1653 24.123 14.566 2.685 1.00 51.50 **ATOM** 1591 CE1 TYR 1653 23.701 13.658 1.724 1.00 53.52 MOTA 1592 CD2 TYR 1653 22.099 14.214 3.917 1.00 52.88 MOTA 1593 CE2 TYR 1653 21.664 13.302 2.966 1.00 54.63 MOTA 1594 CZTYR 1653 22.469 13.025 1.870 1.00 54.35 MOTA 1595 OH TYR 1653 22.049 12.107 0.933 1.00 53.23 MOTA 1597 C TYR 1653 23.717 7.339 16.158 1.00 55.40 MOTA 1598 0 TYR 1653 24.381 15.284 7.900 1.00 54.47 MOTA 1599 N TYR 1654 23.673 17.409 7.773 1.00 MOTA 1601 CA TYR 1654 24.421 17.826 8.947 1.00 58.87 MOTA 1602 CB TYR 1654 24.978 19.235 8.733 1.00 57.91 ATOM 1603 CG TYR 1654 26.068 19.269 7.685 1.00 60.49 MOTA 1604 CD1 TYR 1654 25.760 19.301 6.325 1.00 61.37 MOTA 1605 CE1 TYR 1654 26.769 19.289 5.356 1.00 63.72 MOTA 1606 CD2 TYR 1654 27.412 19.227 8.053 1.00 61.74 MOTA 1607 CE₂ TYR 1654 28.425 19.216 7.099 1.00 64.08 MOTA 1608 CZ TYR 1654 28.102 19.248 5.753 1.00 65.12 MOTA 1609 OH TYR 1654 29.117 19.248 4.817 1.00 64.17 MOTA 1611 C TYR 1654 23.628 17.732 10.245 1.00 60.17 ATOM 1612 O TYR 1654 24.173 17.935 11.335 1.00 61.09 MOTA 1613 N LYS 1655 22.348 17.393 10.133 1.00 60.54 MOTA 1615 CA LYS 1655 21.493 17.277 11.306 1.00 62.12 MOTA 1616 CB LYS 1655 20.019 17.382 10.910 1.00 64.32 MOTA 1617 CG LYS 1655 19.054 17.346 12.079 1.00 67.17 MOTA 1618 CD LYS 1655 17.644 17.608 11.602 1.00 73.05 MOTA 1619 CE LYS 1655 16.626 17.243 12.660 1.00 77.36 MOTA 1620 NZ LYS 1655 15.230 17.494 12.186 1.00 81.10 MOTA 1624 C LYS 1655 21.754 15.976 12.057 1.00 62.19 MOTA 1625 О LYS 1655 21.902 14.907 11.454 1.00 61.36 ATOM 1626 N LYS 1656 21.822 16.084 13.380 1.00 62.26 MOTA 1628 CA LYS 1656 22.069 14.933 14.236 1.00 62.28 MOTA 1629 CB LYS 1656 23.027 15.310 15.372 1.00 62.05 MOTA 1630 CG LYS 1656 24.474 15.489 14.957 62,62 1.00 MOTA 1631 CD LYS 1656 25.320 15.889 16.157 1.00 66.45 MOTA 1632 CE LYS 1656 26.803 15.666 15.908 1.00 67.28 MOTA 1633 LYS NZ. 1656 27.619 16.007 17.109 1.00 68.45 ATOM 1637 С 1656 LYS 20.774 14.381 14.824 1.00 61.86 MOTA 1638 0 LYS 1656 19.714 15.007 14.733 1.00 62.95 MOTA 1639 N 13.198 THR 1657 20.875 15.420 1.00 60.10 ATOM 1641 CA THR 1657 19.743 12.541 16.053 1.00 57.73 MOTA 1642 CB THR 1657 19.973 11.012 16.121 1.00 56.04 MOTA 1643 OG1 THR 1657 21.150 10.730 16.896 1.00 55.21 MOTA 1645 CG2 THR 1657 20.152 10.431 14.731 1.00 53.07 ATOM 1646 C THR 1657 19.664 13.102 17.472 1.00 57.74 MOTA 1647 0 THR 1657 20.513 13.899 17.870 1.00 57.76 MOTA 1648 N THR 1658 18.678 12.667 58.80 18.249 1.00 MOTA 1650 CA THR 1658 18.548 13.140 19.627 1.00 60.33 MOTA 1651 CB THR 1658 17.318 12.517 20.290 1.00 61.37 **ATOM** 1652 C THR 1658 19.811 12.779 20.406 1.00 60.43

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MOTA 1653 0 THR 1658 20.350 13.599 21.155 1.00 60.59 MOTA 1654 N ASN 1659 20.311 11.567 20.161 1.00 59.97 MOTA 1656 CA ASN 1659 21.508 11.058 20.827 1.00 58.28 MOTA 1657 CB ASN 1659 21.607 9.545 20.645 1.00 59.95 MOTA 1658 CG ASN 1659 22.444 8.883 21.723 1.00 60.10 MOTA 1659 OD1 ASN 1659 22.382 9.265 22.891 1.00 61.26 MOTA 1660 ND2 ASN 1659 23.210 7.867 21.341 1.00 57.09 MOTA 1663 С ASN 1659 22.781 11.717 20.311 1.00 57.13 MOTA 1664 0 ASN 1659 23.868 11.418 20.793 1.00 57.34 ATOM 1665 N GLY 1660 22.643 12.570 19.299 1.00 56.48 MOTA 1667 CA GLY 1660 23.781 13.276 18.733 1.00 54.87 MOTA 1668 C GLY 1660 24.539 12.570 17.623 1.00 53.04 MOTA 1669 0 GLY 1660 25.716 12.855 17.394 1.00 54.11 MOTA 1670 N - ARG 1661 -- 23.879 11.659 16.918 1.00 51.37 ATOM 1672 CA ARG 1661 24.536 10.930 15.833 1.00 48.96 MOTA 1673 CB ARG 1661 24.283 9.428 15.961 1.00 48.48 MOTA 1674 CG ARG 8.796 1661 24.848 17.215 1.00 50.03 MOTA 1675 CD ARG 1661 24.492 7.325 17.234 1.00 50.78 MOTA 1676 NE ARG 1661 25.013 6.614 18.396 1.00 50.11 MOTA 1678 CZ ARG 1661 24.902 5.299 18.566 1.00 50.08 MOTA 1679 NH1 ARG 1661 24.286 4.560 17.645 1.00 46.57 MOTA 1682 NH2 ARG 1661 25.426 4.717 19.643 1.00 47.88 MOTA 1685 C 14.459 ARG 1661 24.076 1.00 11.422 46.53 MOTA 1686 0 ARG 1661 23.031 12.029 14.325 1.00 45.01 MOTA 1687 N LEU 1662 24.839 11.094 13.432 1.00 42.39 MOTA 1689 CA LEU 1662 24.546 11.503 12.076 1.00 40.71 **ATOM** 1690 CB LEU 1662 25.823 12.031 11.399 1.00 40.25 MOTA 1691 CG LEU 1662 26.408 13.332 11.965 1.00 42.44 MOTA 1692 CD1 LEU 1662 27.853 13.478 11.537 1.00 40.42 MOTA 1693 CD2 LEU 1662 25.591 14.536 11.514 1.00 41.16 MOTA 1694 С LEU 1662 23.946 10.362 11.258 1.00 38.45 MOTA 1695 O LEU 1662 24.647 9.436 10.862 1.00 36.67 MOTA 1696 N PRO 1663 22.632 10.428 10.987 1.00 37.09 MOTA 1697 CD PRO 1663 21.717 11.475 11.489 1.00 38.18 MOTA 1698 CA PRO 1663 21.894 9.424 10.207 1.00 35.59 MOTA 1699 1663 CB PRO 20.535 10 098 9.983 1.00 35.90 MOTA 1700 CG PRO 1663 20.343 10.856 11.258 1.00 39.13 ATOM 1701 C PRO 1663 22.556 9.045 8.876 1.00 33.05 MOTA 1702 O PRO 1663 22.362 7.933 **B.378** 1.00 31.16 ATOM 1703 N VAL 1664 23.333 9.960 8.299 1.00 32.07 MOTA 1705 CA VAL 1664 24.020 9.669 7.034 1.00 32.49 MOTA 1706 CB VAL 1664 24.831 10.886 6.477 1.00 32.68 MOTA 1707 CG1 VAL 1664 23.898 11.906 5.864 1.00 32.25 MOTA 1708 CG2 VAL 1664 25.670 11.523 7.571 1.00 33.22 MOTA 1709 С VAL 1664 24.957 8.469 7.171 1.00 29.57 MOTA 1710 0 VAL 1664 25.328 7.864 6.175 1.00 27.39 MOTA 1711 N LYS 1665 25.303 8.116 8.409 1.00 28.82 ATOM 1713 CA LYS 1665 26.189 6.991 8.673 1.00 27.87 **ATOM** 1714 CB LYS 1665 26.815 7.100 10.065 1.00 26.99 **ATOM** 1715 CG 1665 LYS 27.967 8.089 10.079 1.00 29.23 **ATOM** 1716 CD LYS 1665 28.283 8.619 11.466 1.00 30.64 **ATOM** 1717 CE LYS 1665 29.543 9.478 11.426 1.00 30.94 MOTA 1718 NZ LYS 1665 29.826 10.128 12.737 1.00 31.63 **ATOM** 1722 С LYS 1665 25.546 5.637 8.465 1.00 26.76

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MOTA 1723 0 LYS 1665 26.211 4.615 8.589 1.00 26.78 **ATOM** 1724 N TRP 1666 24.260 5.630 8.137 1.00 25.79 **ATOM** 1726 CA TRP 1666 23.561 4.381 7.865 1.00 26.56 MOTA 1727 CB TRP 1666 22.299 4.273 8.724 1.00 25.63 MOTA 1728 CG TRP 1666 22.564 3.872 10.174 1.00 26.95 MOTA 1729 CD2 TRP 1666 23.052 4.717 11.232 1.00 24.83 ATOM 1730 CE2 TRP 1666 23.134 3.920 12.398 1.00 24.49 MOTA 1731 CE3 TRP 1666 23.433 6.062 11.306 1.00 24.54 MOTA 1732 CD1 TRP 1666 22.376 2.636 10.730 1.00 20.10 MOTA 1733 NE1 TRP 1666 22.716 2.660 12.063 1.00 21.86 MOTA 1735 CZ2 TRP 1666 23.575 4.433 13.627 1.00 25.71 MOTA 1736 CZ3 TRP 1666 23.870 6.569 12.523 1.00 26.00 **MOTA** 1737 CH2 TRP 1666 23.939 5.754 13.665 1.00 26.04 MOTA 1738 С TRP 1666... 23.188 4.263 6.386 1.00 23.62 MOTA 1739 0 TRP 1666 22.754 3.214 5.931 1.00 24.87 ATOM 1740 N MET 1667 23.404 5.330 5.631 1.00 22.78 MOTA 1742 CA MET 1667 23.046 5.361 4.215 1.00 23.73 **ATOM** 1743 CB MET 1667 22.894 6.802 3.744 1.00 26.24 MOTA 1744 CG 1667 MET 21.823 7.621 4.434 1.00 35.55 MOTA 1745 SD MET 1667 21.795 9.276 3.706 1.00 42.23 ATOM 1746 CE 1667 21.019 MET 8.904 2.238 1.00 40.57 MOTA 1747 C 23.991 MET 1667 4.693 3.239 1.00 22.77 MOTA 1748 O MET 1667 25.205 4.894 3.294 1.00 24.25 MOTA 1749 N ALA 1668 23.420 3.963 2.286 1.00 22.73 ATOM 1751 CA ALA 1668 24.217 3.337 1.237 1.00 23.54 MOTA 1752 CB ALA 1668 23.339 2.495 0.340 1.00 21.80 MOTA 1753 C ALA 1668 24.805 4.495 0.430 1.00 25.53 MOTA 1754 0 ALA 1668 24.181 5.551 0.316 1.00 23.66 MOTA 1755 N PRO 1669 26.006 4.314 -0.153 1.00 26.86 **ATOM** 1756 CD PRO 1669 26.899 3.144 -0.095 1.00 26.35 ATOM 1757 CA PRO 1669 26.611 5.390 -0.942 1.00 27.78 ATOM 1758 CB PRO 4.731 1669 27.864 -1.518 1.00 25.51 MOTA 1759 CG PRO 1669 28.225 3.741 -0.471 1.00 25.36 MOTA 1760 С PRO 1669 25.686 5.900 -2.057 1.00 26.47 MOTA 1761 0 PRO 1669 25.617 7.099 -2.288 1.00 28.42 ATOM 1762 N GLU 1670 24.951 5.010 -2.724 1.00 26.88 MOTA 1764 CA GLU 1670 24.057 5.459 -3.796 1.00 29.03 MOTA 1765 CB GLU 1670 23.597 4.293 -4.693 1.00 31.79 MOTA 1766 CG GLU 1670 22.588 3.325 -4.065 1.00 32.47 MOTA 1767 CD **GLU** 1670 23.212 2.184 -3.255 1.00 32.43 MOTA 1768 OE1 GLU 1670 22.429 1.297 -2.822 1.00 25.01 MOTA 1769 OE2 GLU 1670 24.458 2.157 -3.069 1.00 28.75 ATOM 1770 С GLU 1670 22.864 6.274 -3.294 1.00 28.37 MOTA 1771 0 GLU 1670 22.358 7.146 -4.001 1.00 25.72 MOTA 1772 N ALA 1671 22.451 6.028 -2.053 1.00 30.08 MOTA 1774 CA ALA 1671 21.347 6.779 -1.465 1.00 31.24 MOTA 1775 CB ALA 1671 20.751 6.031 -0.287 1.00 26.42 MOTA 1776 С ALA 1671 21.899 8.125 -1.013 1.00 31.36 MOTA 1777 0 ALA 1671 21.298 9.167 -1.249 1.00 33.11 MOTA 1778 N LEU 1672 23.068 8.096 -0.387 1.00 32.73 MOTA 1780 CA LEU 1672 23.715 9.304 0.100 1.00 33.96 MOTA 1781 CB LEU 1672 24.931 8.935 0.940 1.00 33.89 MOTA 1782 CG LEU 1672 25.783 10.071 1.502 1.00 37.62 MOTA 1783 CD1 LEU 1672 25.010 10.800 2.581 1.00 39.57

MOTA	1784	CD2	LEU	1672	27.054	9.491	2.087	1.00	32.30
ATOM	1785	С	LEU	1672	24.157	10.207	-1.042	1.00	36.83
MOTA	1786	0	LEU	1672	23.769	11.369	-1.102	1.00	37.87
MOTA	1787	N	PHE	1673	24.959	9.669	-1.954	1.00	35.82
MOTA	1789	CA	PHE	1673	25.466	10.449	-3.071	1.00	35.82
ATOM	1790	CB	PHE	1673	26.738	9.802	-3.639	1.00	34.66
ATOM	1791	CG	PHE	1673	27.850	9.642	-2.634	1.00	33.84
ATOM	1792	CD1	PHE	1673	28.503	8.422	-2.494	1.00	32.65
MOTA	1793	CD2	PHE	1673	28.242	10.709	-1.827	1.00	36.98
ATOM	1794	CE1	PHE	1673	29.540	8.257	-1.555	1.00	37.95
MOTA	1795	CE2	PHE	1673	29.279	10.557	-0.881	1.00	39.90
ATOM	1796	CZ	PHE	1673	29.927	9.325	-0.748	1.00	37.09
ATOM	1797	С	PHE	167 3	24.483	10.692	-4.210	1.00	36.34
MOTA	1798	0	PHE	1673	24.430	11.788	-4.754	1:00	37.18
MOTA	1799	N	ASP	1674	23.705	9.677	-4.568	1.00	38.22
MOTA	1801	CA	ASP	1674	22.780	9.777	-5.693	1.00	38.51
ATOM	1802	CB	ASP	1674	23.008	8.597	-6.633	1.00	40.34
MOTA	1803	CG	ASP	1674	24.439	8.511	-7.122	1.00	43.87
ATOM	1804	OD1	ASP	1674	25.092	9.571	-7.254	1.00	42.79
MOTA	1805	OD2	ASP	1674	24.906	7.376	-7.369	1.00	47.94
ATOM	1806	С	ASP	1674	21.298	9.853	-5.360	1.00	40.21
ATOM	1807	0	ASP	1674	20.457	9.872	-6.271	1.00	39.07
ATOM	1808	N	ARG	1675	20.975	9.836	-4.072	1.00	39.83
MOTA	1810	CA	ARG	1675	19.589	9.900	-3.631	1.00	42.25
ATOM	1811	CB	ARG	1675	18.992	11.271	-3.964	1.00	48.19
ATOM	1812	CG	ARG	1675	19.691	12.420	-3.267	1.00	59.20
MOTA	1813	CD	ARG	1675	19.462	13. 7 29	-4.019	1.00	67.81
MOTA	1814	NE	ARG	1675	20.079	14.876	-3.352	1.00	75.11
ATOM	1816	CZ	ARG	1675	19.688	16.136	-3.525	1.00	78.74
ATOM	1817	NH1	ARG	1675	18.680	16.429	-4.341	1.00	79.91
ATOM	1820	NH2	ARG	1675	20.311	17.115	-2.890	1.00	81.24
MOTA	1823	С	ARG	1675	18.730	8.777	-4.221	1.00	39.00
MOTA	1824	0	ARG	1675	17.544	8.956	-4.488	1.00	39.71
ATOM	1825	N	ILE	1676	19.345	7.624	-4.434	1.00	35.50
ATOM	1827	CA	ILE	1676	18.636	6.471	-4.958	1.00	33.51
ATOM	1828	CB	ILE	1676	19.434	5.759	-6.039	1.00	34.59
ATOM	1829	CG2	ILE	1676	18.582	4.678	-6.649	1.00	33.90
ATOM	1830	CG1	ILE	1676	19.848	6.752	-7.120	1.00	37.60
MOTA	1831	CD1	ILE	1676	20.861	6.197	-8.109	1.00	42.67
ATOM	1832	C	ILE	1676	18.390	5.501	-3.809	1.00	30.94
MOTA	1833	0	ILE	1676	19.326	4.926	-3.252	1.00	28.62
ATOM	1834	N	TYR	1677	17.124	5.351	-3.443	1.00	30.60
ATOM	1836	CA	TYR	1677	16.724	4.467	-2.359	1.00	25.87
ATOM	1837	CB	TYR	1677	15.781	5.197	-1.413	1.00	26.40
ATOM	1838	CG	TYR	1677	16.483	6.220	-0.555	1.00	27.67
ATOM	1839	CD1	TYR	1677	16.663	7.533	-0.999	1.00	27.45
ATOM	1840	CE1	TYR	1677	17.269	8.483	-0.191	1.00	26.55
ATOM	1841	CD2	TYR	1677	16.935	5.883	0.721	1.00	24.58
MOTA	1842	CE2	TYR	1677	17.536	6.828	1.538	1.00	26.35
ATOM	1843	CZ	TYR	1677	17.698	8.122	1.080	1.00	28.80
ATOM	1844	ОН	TYR	1677	18.270	9.059	1.914	1.00	34.97
MOTA	1846	C	TYR	1677	16.055	3.235	-2.911	1.00	22.70
ATOM	1847	0	TYR	1677	15.144	3.335	-3.728	1.00	26.22
ATOM	1848	N	THR	1678	16.477	2.076	-2.420	1.00	21.83

ATOM	1850	CA	THR	1678	15.968	0.791	-2.865	1.00	22.14
ATOM	1851	CB	THR	1678	16.907	0.191	-3.928	1.00	23.91
ATOM	1852	OG1	THR	1678	18.229	0.105	-3.373	1.00	27.47
ATOM	1854	CG2	THR	1678	16.949	1.053	-5.188	1.00	24.94
ATOM	1855	C	THR	1678	15.999	-0.176	-1.692	1.00	22.79
ATOM	1856	0	THR	1678	16.427	0.170	-0.592	1.00	23.39
ATOM	1857	N	HIS	1679	15.563	-1.402	-1.929	1.00	21.98
ATOM	1859	CA	HIS	1679	15.613	-2.417	-0.888	1.00	22.97
MOTA	1860	CB	HIS	1679	14.872	-3.671	-1.351	1.00	22.04
MOTA	1861	CG	HIS	1679	13.421	-3.444	-1.621	1.00	25.41
MOTA	1862	CD2	HIS	1679	12.674	-3.611	-2.740	1.00	26.60
ATOM	1863	ND1	HIS	1679	12.556	-2.954	-0.663	1.00	26.13
MOTA	1865	CEl	HIS	1679	11.348	-2.830	-1.178	1.00	28.66
MOTA	1866	NE2	HIS	1679	11.394	-3.221	-2.441	1.00	29.66
ATOM	1868	C	HIS	1679	17.097	-2.719	-0.650	1.00	23.14
ATOM	1869	0	HIS	1679	17.511	-3.074	0.459	1.00	21.69
ATOM	1870	N	GLN	1680	17.895	-2.506	-1.697	1.00	22.38
ATOM	1872	CA	GLN	1680	19.335	-2.726	-1.658	1.00	22.33
ATOM	1873	СВ	GLN	1680	19.948	-2.594	~3.058	1.00	22.52
MOTA	1874	CG	GLN	1680	19.895	-3.872	-3.879	1.00	29.15
ATOM	1875	CD	GLN	1680	18.865	-3.847	-4.991	1.00	33.60
ATOM	1876	OE1	GLN	1680	17.819	-3.212	-4.871	1.00	38.43
ATOM	1877	NE2	GLN	1680	19.159	-4.542	-6.085	1.00	33.44
ATOM	1880	С	GLN	1680	20.007	-1.740	-0.732	1.00	22.61
MOTA	1881	0	GLN	1680	20.943	-2.093	-0.027	1.00	22.00
ATOM	1882	N	SER	1681	19.562	-0.490	-0.745	1.00	22.06
ATOM	1884	CA	SER	1681	20.184	0.479	0.137	1.00	23.41
ATOM	1885	СВ	SER	1681	19.886	1.923	-0.306	1.00	20.06
ATOM	1886	OG	SER	1681	18.503	2.166	-0.479	1.00	22.90
ATOM	1888	С	SER	1681	19.778	0.206	1.583	1.00	23.08
ATOM	1889	0	SER	1681	20.528	0.531	2.506	1.00	24.13
MOTA	1890	N	ASP	1682	18.608	-0.412	1.770	1.00	23.19
MOTA	1892	CA	ASP	1682	18.107	-0.775	3.104	1.00	22.37
MOTA	1893	CB	ASP	1682	16.660	-1.275	3.018	1.00	24.55
MOTA	1894	CG	ASP	1682	15.616	-0.172	3.222	1.00	24.22
MOTA	1895	OD1	ASP	1682	14.428	-0.479	3.005	1.00	25.02
MOTA	1896	OD2	ASP	1682	15.949	0.968	3.625	1.00	24.82
MOTA	1897	С	ASP	1682	18.980	-1.888	3.690	1.00	20.47
ATOM	1898	0	ASP	1682	19.172	-1.984	4.906	1.00	21.83
ATOM	1899	N	VAL	1683	19.480	-2.746	2.806	1.00	20.14
ATOM	1901	CA	VAL	1683	20.340	-3.856	3.179	1.00	20.49
ATOM	1902	CB	VAL	1683	20.493	-4.842	2.003	1.00	22.38
MOTA	1903	CG1	VAL	1683	21.757	-5.691	2.159	1.00	19.57
MOTA	1904	CG2	VAL	1683	19.264	-5.740	1.942	1.00	22.35
MOTA	1905	C	VAL	1683	21.677	-3.315	3.683	1.00	20.22
MOTA	1906	0	VAL	1683	22.202	-3.789	4.684	1.00	21.41
ATOM	1907	N	TRP	1684	22.210	-2.311	3.003	1.00	21.33
ATOM	1909	CA	TRP	1684	23.440	-1.666	3.449	1.00	22.21
MOTA	1910	СВ	TRP	1684	23.768	-0.473	2.540	1.00	18.78
ATOM	1911	CG	TRP	1684	24.924	0.391	3.037	1.00	22.80
ATOM	1912	CD2	TRP	1684	26.237	0.477	2.472	1.00	24.60
MOTA	1913	CE2	TRP	1684	26.989	1.364	3.286	1.00	24.34
ATOM	1914	CE3	TRP	1684	26.853	-0.099	1.352	1.00	24.34
ATOM	1915	CD1	TRP	1684	24.933	1.208	4.138	1.00	22.28
									0

ATOM	1916	NE1	TRP	1684	26.169	1.791	4.297	1.00	22.32
ATOM	1918	CZ2	TRP	1684	28.324	1.669	3.022	1.00	24.77
ATOM	1919	CZ3	TRP	1684	28.193	0.213	1.090	1.00	24.46
ATOM	1920	CH2	TRP	1684	28.906	1.088	1.918	1.00	24.00
MOTA	1921	С	TRP	1684	23.198	-1.183	4.899	1.00	23.26
MOTA	1922	0	TRP	1684	23.982	-1.475	5.805	1.00	24.52
MOTA	1923	N	SER	1685	22.108	-0.447	5.113	1.00	22.88
MOTA	1925	CA	SER	1685	.21.744	0.057	6.444	1.00	24.01
MOTA	1926	CB	SER	1685	20.398	0.783	6.385	1.00	21.90
MOTA	1927	OG	SER	1685	20.424	1.787	5.388	1.00	24.75
ATOM	1929	С	SER	1685	21.659	-1.087	7.464	1.00	24.28
ATOM	1930	0	SER	1685	22.077	-0.933	8.625	1.00	23.94
ATOM	1931	N	PHE	1686	21.099	-2.221	7.037	1.00	23.20
ATOM	1933	CA	PHE	1686	20.993	-3.393	7.898	1.00	23.87
ATOM	1934	СВ	PHE	1686	20.216	-4.519	7.216	1.00	19.56
ATOM	1935	CG	PHE	1686	20.062	-5.734	8.075	1.00	22.19
ATOM	1936	CD1	PHE	1686	19.240	-5.701	9.203	1.00	21.55
ATOM	1937	CD2	PHE	1686	20.773	-6.899	7.793	1.00	21.94
ATOM	1938	CE1	PHE	1686	19.125	-6.801	10.033	1.00	21.66
ATOM	1939	CE2	PHE	1686	20.663	-8.012	8.623	1.00	22.47
ATOM	1940	CZ	PHE	1686	19.842	-7.961	9.743	1.00	23.14
ATOM	1941	С	PHE	1686	22.389	-3.890	8.300	1.00	22.62
ATOM	1942	0	PHE	1686	22.579	-4.424	9,407	1.00	23.09
ATOM	1943	N	GLY	1687	23.354	-3.726	7.401	1.00	23.50
ATOM	1945	CA	GLY	1687	24.718	-4.110	7.721	1.00	23.83
ATOM	1946	С	GLY	1687	25.230	-3.247	8.867	1.00	21.95
ATOM	1947	0	GLY	1687	25.901	-3.749	9.778	1.00	23.76
ATOM	194B	N	VAL	1688	24.928	-1.947	8.817	1.00	20.60
ATOM	1950	CA	VAL	1688	25.331	-1.009	9.877	1.00	22.34
MOTA	1951	СВ	VAL	1688	25.020	0.481	9.488	1.00	20.94
MOTA	1952	CG1	VAL	1688	25.547	1.438	10.543	1.00	21.65
ATOM	1953	CG2	VAL	1688	25.675	0.832	8.160	1.00	22.71
MOTA	1954	С	VAL	1688	24.598	-1.400	11.182	1.00	22.71
ATOM	1955	0	VAL	1688	25.199	-1.479	12.255	1.00	22.78
ATOM	1956	N	LEU	1689	23.310	-1.706	11.082	1.00	22.81
ATOM	1958	CA	LEU	1689	22.534	-2.111	12.253	1.00	25.21
ATOM	1959	СВ	LEU	1689	21.064	-2.357	11.866	1.00	25.78
ATOM	1960	CG	LEU	1689	20.006	-2.491	12.976	1.00	29.18
MOTA	1961	CD1	LEU	1689	18.643	-2.109	12.408	1.00	28.57
ATOM	1962	CD2	LEU	1689	19.959	-3.895	13.553	1.00	26.77
MOTA	1963	C	LEU	1689	23.158		12.871		25.88
ATOM	1964	0	LEU	1689	23.249	-3.483	14.099	1.00	26.50
ATOM	1965	N	LEU	1690	23.588	-4.323	12.031	1.00	25.84
ATOM	1967	CA	LEU	1690	24.221	-5.544	12.523	1.00	24.43
ATOM	1968	CB	LEU	1690	24.669	-6.444	11.377	1.00	26.35
MOTA	1969	CG	LEU	1690	23.672	-7.309	10.604	1.00	26.57
ATOM	1970	CD1	LEU	1690	24.415	-7.962	9.446	1.00	26.33
ATOM	1971	CD2	LEU	1690	23.042	-8.380	11.502	1.00	24.66
ATOM	1972	C	LEU	1690	25.430	-5.168	13.349	1.00	25.22
ATOM	1973	ō	LEU	1690	25.646	-5.706	14.435	1.00	24.84
ATOM	1974	N	TRP	1691	26.211	-4.227	12.826	1.00	26.92
ATOM	1976	CA	TRP	1691	27.405	-3.728	13.504	1.00	25.77
ATOM	1977	СВ	TRP	1691	28.072	-2.659	12.631	1.00	24.82
ATOM	1978	CG	TRP	1691	29.394	-2.195	13.154	1.00	27.98
			/.			در د	AJ. AJ3	1.00	21.30

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ATOM 1979 CD2 TRP 1691 29.623 -1.104 14.056 1.00 26.95 **ATOM** 1980 CE2 TRP 1691 31.022 -1.015 14.259 1.00 27.64 MOTA 1981 CE3 TRP 1691 28.783 -0.191 14.708 1.00 26.28 MOTA 1982 CD1 TRP 1691 30.634 -2.715 12.856 1.00 28.38 MOTA 1983 NE1 31.609 -2.009 TRP 1691 13.518 1.00 29.56 MOTA 1985 CZ.2 TRP 1691 31.599 -0.045 15.086 1.00 27.78 MOTA 1986 CZ3 TRP 1691 29.356 0.769 15.533 1.00 27.63 MOTA 1987 CH2 TRP 30.753 1691 0.835 15.713 1.00 30.68 MOTA 1988 TRP С 1691 27.025 -3.147 14.876 1.00 26.38 MOTA 1989 0 TRP 1691 27.686 -3.414 15.883 1.00 24.82 1990 MOTA N GLU 1692 25.926 -2.393 14.916 1.00 27.62 MOTA 1992 CA GLU 1692 25.442 -1.790 16.162 1.00 27.02 MOTA 1993 CB 24.193 GLU 1692 -0.963 15.919 29.27 1.00 ATOM . 1994 CG GLU 1692 24:345 0.236 15.028 1.00 24.77 MOTA 1995 CD 23.046 GLU 1692 0.992 14.962 1.00 25.98 MOTA 1996 OE1 GLU 1692 22.238 0.694 14.058 1.00 22.29 MOTA 1997 OE2 GLU 1692 22.803 1.837 15.850 1.00 25.12 MOTA 1998 C GLU 1692 25.092 -2.856 17.191 1.00 27.88 MOTA 1999 0 GLU 1692 25.333 -2.673 18.379 1.00 30.18 MOTA 2000 N ILE 1693 24.500 -3.956 16.734 1.00 26.65 MOTA 2002 CA ILE 1693 24.118 -5.054 17.618 1.00 26.14 MOTA 2003 CB ILE 1693 23.279 -6.144 16.858 1.00 25.37 MOTA 2004 CG2 ILE 1693 23.144 -7.445 17.704 1.00 21.48 MOTA 2005 CG1 ILE 1693 21.897 -5.563 1.00 16.496 24.80 MOTA 2006 CD1 ILE 1693 21.017 -6.479 15.642 1.00 22.40 MOTA 2007 С ILE 1693 25.345 -5.698 18.239 1.00 27.17 MOTA 2008 С ILE 1693 25.424 -5.864 19.452 1.00 27.30 ATOM 2009 N PHE 1694 26.329 -6.017 17.414 1.00 29.98 2011 MOTA CA PHE 1694 27.518 -6.674 17.925 1.00 30.61 MOTA 2012 CB PHE 1694 28.140 -7.556 16.843 1.00 28.30 MOTA 2013 CG PHE 1694 27.197 -8.611 16.353 1.00 30.91 MOTA 2014 CD1 PHE 1694 26.627 -8.526 15.088 1.00 34.46 MOTA 2015 CD2 PHE 1694 26.743 -9.601 17.224 1.00 32.71 MOTA 2016 CE1 PHE 1694 25.622 -9.409 14.701 1.00 34.24 MOTA 2017 CE₂ PHE 1694 25.737 -10.490 1.00 16.844 32.44 MOTA 2018 CZPHE 1694 25.170 -10.387 15.592 1.00 32.70 MOTA 2019 C PHE 1694 28.512 -5.796 18.689 1.00 31.74 MOTA 2020 O PHE 1694 29.469 -6.299 19.276 1.00 35.15 MOTA 2021 28.275 N THR 1695 -4.489 18.698 1.00 31.12 MOTA 2023 CA THR 1695 29.101 -3.575 19.473 1.00 29.96 MOTA 2024 CB THR 1695 29.532 -2.351 18.657 1.00 28.09 **ATOM** 2025 OG1 THR 1695 28.373 -1.685 18.150 1.00 30.65 MOTA 2027 CG2 THR 1695 30.450 -2.767 17.510 1.00 23.37 MOTA 2028 C THR 1695 28.240 -3.128 20.664 1.00 30.01 ATOM 2029 0 1695 THR 28.617 -2.233 21,427 1.00 31.14 MOTA 2030 N LEU 1696 27.078 -3.766 20.797 1.00 27.96 MOTA 2032 CA LEU 1696 26.113 -3.490 21.862 1.00 30.25 **ATOM** 2033 CB 1696 23.216 LEU 26.633 -3.985 1.00 33.54 2034 MOTA CG LEU 1696 26.899 -5.482 1.00 23.339 32.61 MOTA 2035 CD1 LEU 1696 27.473 -5.777 24.711 1.00 33.54 **ATOM** 2036 CD2 LEU 1696 25.602 -6.233 23.126 1.00 36.37 MOTA 2037 С LEU 1696 25.717 -2.031 21.958 1.00 28.19 MOTA 2038 0 LEU 1696 25.792 -1.431 23.018 1.00 29.18 **ATOM** 2039 N GLY 1697 25.251 -1.472 20.853 1.00 28.24

ATOM	2041	CA	GLY	1697	24.851	-0.082	20.858	1.00	28.29
ATOM	2042	С	GLY	1697	25.990	0.845	20.499	1.00	27.68
ATOM	2043	0	GLY	1697	25.960	2.022	20.846	1.00	29.79
ATOM	2044	N	GLY	1698	26.986	0.324	19.790	1.00	29.23
ATOM	2046	CA	GLY	1698	28.115	1.143	19.396	1.00	30.79
ATOM	2047	C	GLY	1698	27.743	2.212	18.388	1.00	32.38
MOTA	2048	0	GLY	1698	26.817	2.044	17.601	1.00	33.26
ATOM	2049	N	SER	1699	28.480	3.314	18.411	1.00	30.81
ATOM	2051	CA	SER	1699	28.268	4.437	17.510	1.00	32.03
ATOM	2052	СВ	SER	1699	28.528	5.728	18.288	1.00	34.81
ATOM	2053	OG	SER	1699	28.559	6.862	17.440	1.00	40.03
ATOM	2055	c	SER	1699	29.198	4.325	16.282	1.00	32.20
ATOM	2056	0	SER	1699	30.428	4.325	16.408	1.00	31.67
ATOM	2057	N	PRO	1700	28.620		15.082	1.00	32.62
ATOM	2058	CD	PRO	1700	27.178	4.142	14.773	1.00	34.19
ATOM	2059	CA	PRO	1700	29.422	4.028	13.856	1.00	31.76
ATOM	2060	СВ	PRO	1700	28.357	3.830	12.759	1.00	32.04
ATOM	2061	CG	PRO	1700	27.145	3.351	13.502	1.00	
MOTA	2062	C	PRO	1700	30.214	5.309			33.17
ATOM	2063	0	PRO	1700	29.715	6.391	13.609	1.00	28.70
ATOM	2064	N	TYR	1701	31.459	5.181	13.871 13.164	1.00	28.57
ATOM	2066	CA	TYR	1701	32.311			1.00	28.61
ATOM	2067	CB			32.311	6.338	12.870	1.00	29.92
MOTA	2068	CG	TYR	1701		6.946	11.510	1.00	30.15
ATOM	2068	CD1	TYR	1701	31.965	5.994	10.339	1.00	36.17
ATOM	2070	CE1	TYR TYR	1701	30.799 ,	5.630 4.767	9.664	1.00	39.26
ATOM	2071	CD2	TYR	1701	30.839		8.571	1.00	41.51
ATOM	2071	CE2		1701	33.176	5.467	9.893	1.00	37.48
ATOM	2072	CZ	TYR TYR	1701	33.229	4.607	8.805	1.00	42.94
ATOM				1701	32.059	4.263	8.146	1.00	45.72
ATOM	2074 2076	OH C	TYR	1701	32.110	3.431	7.043	1.00	53.99
			TYR	1701	32.279	7.448	13.941	1.00	31.09
MOTA	2077	0	TYR	1701	31.935	8.592	13.649	1.00	31.93
MOTA MOTA	2078	N	PRO	1702	32.649	7.135	15.189	1.00	34.66
ATOM	2079	CD	PRO	1702	33.212	5.879	15.708	1.00	36.83
	2080	CA	PRO	1702	32.631	8.173	16.231	1.00	33.54
ATOM	2081	CB	PRO	1702	33.116	7.432	17.479	1.00	32.18
ATOM	2082	CG	PRO	1702	32.903	6.001	17.175	1.00	40.82
ATOM ATOM	2083	C	PRO	1702	33.628	9.274	15.883	1.00	34.78
	2084	0	PRO	1702	34.750	8.981	15.455	1.00	33,97
MOTA MOTA	2085	N	GLY	1703	33.220	10.528	16.074	1.00	36.45
	2087	CA	GLY	1703	34.085		15.788	1.00	34.40
MOTA	2088	C	GLY	1703	34.245	12.006	14.317	1.00	34.34
MOTA	2089	0	GLY	1703	34.977	12.933	13.969	1.00	34.20
ATOM	2090	N	VAL	1704	33.552	11.275	13.445	1.00	35.02
ATOM	2092	CA	VAL	1704	33.641	11.512	12.007	1.00	32.77
MOTA	2093	CB	VAL	1704	33.614	10.176	11.221	1.00	31.32
ATOM	2094		VAL	1704	33.628	10.435	9.709	1.00	31.46
MOTA	2095	CG2	VAL	1704	34.796	9.297	11.637	1.00	27.62
MOTA	2096	С	VAL	1704	32.510	12.410	11.513	1.00	33.35
MOTA	2097	0	VAL	1704	31.337	12.070	11.640	1.00	33.94
ATOM	2098	N	PRO	1705	32.849	13.589	10.974	1.00	32.43
MOTA	2099	CD	PRO	1705	34.181	14.221	10.949	1.00	32.77
MOTA	2100	CA	PRO	1705	31.826	14.505	10.472	1.00	33.61
MOTA	2101	CB	PRO	1705	32.545	15.853	10.509	1.00	33.21

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MOTA 2102 1705 CG PRO 33.935 15.482 10.141 1.00 35.53 MOTA 2103 PRO С 1705 31.395 14.138 9.052 1.00 33.91 MOTA 2104 0 PRO 1705 32.113 13.409 8.354 1.00 32.65 ATOM 2105 N VAL 1706 30.255 14.684 8.619 1.00 33.82 ATOM 2107 CA VAL 1706 29.689 14.447 7.280 1.00 33.97 **MOTA** 2108 CB VAL 1706 28.617 15.513 6.943 1.00 37.41 ATOM 2109 CG1 VAL 1706 28.045 15.282 5.556 1.00 41.12 MOTA 2110 CG2 VAL 1706 27.507 15.484 7.971 1.00 38.89 MOTA 2111 С VAL 1706 30.712 14.428 6.135 1.00 32.32 MOTA 2112 0 VAL 1706 30.819 13.450 5.398 1.00 32.58 MOTA 2113 N GLU 1707 31.477 15.504 6.004 1.00 31.15 MOTA 2115 CA GLU 1707 32.478 15.630 4.956 1.00 29.82 MOTA 2116 CB GLU 1707 33.172 16.989 5.048 1.00 30.05 MOTA 2117 С GLU 1707 .33.531 14.541 4.959 1.00 28.52 MOTA 2118 0 GLU 1707 33.995 14.134 3.896 1.00 30.85 MOTA 2119 N GLU 1708 33.958 14.110 6.143 1.00 28.70 MOTA 2121 CA GLU 6.235 1708 34.978 1.00 13.073 29.50 MOTA 2122 CB GLU 1708 35.590 13.010 7.641 1.00 31.28 **ATOM** 2123 CG GLU 1708 36.281 8.103 14.289 1.00 41.63 MOTA 2124 CDGLU 1708 37.454 14.718 7.237 1.00 49.91 ATOM 2125 OE1 GLU 1708 38.020 13.876 6.498 1.00 53.57 MOTA 2126 OE2 GLU 1708 37.821 15.916 7.308 1.00 58.45 ATOM 2127 С GLU 1708 34.365 11.730 5.878 1.00 30.00 MOTA 2128 0 GLU 1708 35.016 10.874 5.257 1.00 28.43 33.103 MOTA 2129 N LEU 1709 11.559 6.257 1.00 30.08 MOTA 2131 CA 1709 32.392 LEU 10.324 5.964 1.00 29.19 MOTA 2132 CB LEU 1709 30.995 10.347 6.592 1.00 28.97 MOTA 2133 CG LEU 1709 30.109 9.186 6.137 1.00 30.66 MOTA 2134 CD1 LEU 1709 30.664 7.866 6.659 1.00 29.24 MOTA 2135 CD2 LEU 1709 28.684 9.403 6.593 1.00 29.29 **ATOM** 2136 C LEU 1709 32.294 10.130 4.449 1.00 28.26 **ATOM** 2137 0 LEU 1709 32.450 9.011 3.948 1.00 28.86 ATOM 2138 N PHE 1710 32.016 11.220 3.735 1.00 26.86 MOTA 2140 CA PHE 1710 31.903 11.192 2.285 1.00 28.86 MOTA 2141 CB PHE 1710 31.632 12.593 1.743 1.00 31.88 ATOM 2142 CG PHE 1710 30.249 13.095 2.014 1.00 37.62 ATOM 2143 CD1 PHE 1710 29.265 12.247 2.509 1.00 42.63 MOTA 2144 CD2 PHE 1710 29.931 14.424 1.792 1.00 43.53 MOTA 2145 CE1 PHE 1710 27.977 12.718 2.783 1.00 45.99 ATOM 2146 CE2 PHE 1710 28.648 14.905 2.061 1.00 46.25 MOTA 2147 CZ PHE 1710 27.670 14.045 2.559 1.00 44.45 MOTA 2148 C PHE 1710 33.193 10.660 1.681 1.00 30.42 **MOTA** 2149 0 PHE 1710 33.174 9.807 0.792 1.00 29.01 MOTA 2150 N LYS 1711 34.309 11.152 2.212 1.00 30.64 MOTA 2152 CA LYS 1711 35.650 10.762 1.786 1.00 32.89 MOTA 2153 CB LYS 1711 36.670 11.655 2.502 1.00 37.91 MOTA 2154 CG LYS 1711 38.108 11.479 2.088 1.00 42.99 MOTA 2155 CDLYS 1711 38.976 12.528 2.752 1.00 47.45 MOTA 2156 CE LYS 1711 40.380 12.505 2.182 1.00 52.35 MOTA 2157 NZ LYS 1711 41.104 11.272 2.587 1.00 58.47 MOTA 2161 С LYS 1711 35.913 9.273 2.071 1.00 32.23 MOTA 2162 0 1.00 LYS 1711 36.445 8.559 1.216 30.79 MOTA 2163 N LEU 1712 35.533 B.807 1.00 3.264 31.37 MOTA 2165 CA LEU 1712 35.704 7.399 3.630 1.00 29.46

ATOM	2166	CB	LEU	1712	35.220	7.117	5.065	1.00	28.57
MOTA	2167	CG	LEU	1712	36.045	7.662	6.242	1.00	30.18
MOTA	2168	CD1	LEU	1712	35.395	7.349	7.569	1.00	26.92
MOTA	2169	CD2	LEU	1712	37.452	7.083	6.210	1.00	30.88
MOTA	2170	С	LEU	1712	34.922	6.539	2.651	1.00	28.99
ATOM	2171	0	LEU	1712	35.438	5.551	2.136	1.00	30.73
ATOM	2172	N	LEU	1713	33.675	6.915	2.388	1.00	30.13
ATOM	2174	CA	LEU	1713	32.851	6.158	1.456	1.00	32.10
ATOM	2175	СВ	LEU	1713	31.411	6.685	1.443	1.00	35.23
ATOM	2176	CG	LEU	1713	30.612	6.292	2.691	1.00	37.47
ATOM	2177	CD1	LEU	1713	29.265	6.982	2.720	1.00	40.85
ATOM	2178	CD2	LEU	1713	30.447	4.788	2.723	1.00	39.61
MOTA	2179	C	LEU	1713	33.441	6.147	Ö.047	1.00	32.70
ATOM	-2180		LEU	1713	33.548	5.090	-0.578	1.00	31.86
MOTA	2181	N	LYS	1714	33.859	7.309	-0.444	1.00	
ATOM	2183	CA	LYS	1714	34.440	7.387	-1.776	1.00	32.42
ATOM	2184	СВ	LYS	1714	34.826	8.824		1.00 41.00	32.56
ATOM	2185	CG	LYS	1714	33.640	9.736	-2.297	<u> </u>	33.02
ATOM	2186	CD	LYS	1714	32.736	9.235	-2.297	1.00	35.56
ATOM	2187	CE	LYS	1714	31.635	10.246	-3.682	1.00	37.94
ATOM	2188	NZ	LYS	1714	30.727	9.805	-3.002 -4.779		42.57
ATOM	2192	C	LYS	1714	35.664	6.488	-1.885	1.00 1.00	47.40
ATOM	2193	o	LYS	1714	35.927	5.898	-2.937	1.00	35.36
MOTA	2194	N	GLU	1715	36.376	6.338	-0.775	1.00	36.68
MOTA	2196	CA	GLU	1715	37.577	5.527	-0.749		34.51
ATOM	2197	СВ	GLU	1715	38.566	6.125	0.250	1.00	35.31
ATOM	2198	CG	GLU	1715	38.967	7.537		1.00	37.07
ATOM	2199	CD	GLU	1715	39.735	8.310	-0.163 0.893	1.00	43.62
ATOM	2200	OE1	GLU	1715	39.906	7.814	2.029	1.00 1.00	49.75
ATOM	2201	OE2	GLU	1715	40.163	9.442	0.572	1.00	49.71
ATOM	2202	C	GLU	1715	37.321	4.048	-0.487	1.00	55.13
ATOM	2203	o	GLU	1715	38.259	3.260	-0.438	1.00	34.08 34.82
ATOM	2204	N	GLY	1716	36.049	3.674	-0.366	1.00	31.53
ATOM	2206	CA	GLY	1716	35.695	2.288	-0.133	1.00	27.58
ATOM	2207	C	GLY	1716	35.966	1.765	1.262	1.00	28.60
ATOM	2208	0	GLY	1716	36.069	0.560	1.464	1.00	27.81
ATOM	2209	N	HIS	1717	36.062	2.663	2.236	1.00	29.10
ATOM	2211	CA	HIS	1717	36.319	2.263	3.617	1.00	29.30
ATOM	2212	СВ	HIS	1717	36.501	3.510	4.486	1.00	30.54
ATOM	2213	CG	HIS	1717	36.788	3.213	5.930	1.00	32.88
ATOM	2214	CD2	HIS	1717	37.961	3.023	6.586	1.00	32.21
MOTA	2215	ND1	HIS	1717	35.798	3.108	6.881	1.00	34.22
MOTA	2217	CE1	HIS	1717	36.342	2.865	8.061	1.00	31.51
ATOM	2218	NE2	HIS	1717	37.651	2.809	7.907	1.00	31.94
ATOM	2220	C	HIS	1717	35.180	1.416	4.183	1.00	28.42
ATOM	2221	0	HIS	1717	34.017	1.666	3.885	1.00	
ATOM	2222	N	ARG	1718	35.526	0.450	5.02B	1.00	30.71
ATOM	2224	CA	ARG	1718	34.559	-0.423	5.688	1.00	27.75
ATOM	2225	СВ	ARG	1718	34.562	-1.813	5.048	1.00	27.58
ATOM	2226	CG	ARG	1718	34.078	-1.860	3.597	1.00	29.07 28.39
ATOM	2227	CD	ARG	1718	32.609	-1.412	3.475		
ATOM	2228	NE	ARG	1718	32.091	-1.412		1.00	27.64
ATOM	2230	CZ	ARG	1718			2.096	1.00	24.37
ATOM	2231	NH1	ARG	1718	32.173	-0.476	1.210	1.00	24.26
	4491	*4***	AAG	T / T O	32.768	0.668	1.532	1.00	23.98

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MOTA 2234 -0.603 NH2 ARG 1718 31.595 0.019 1.00 21.60 **ATOM** 2237 C ARG -0.521 1718 35.005 7.148 1.00 30.11 MOTA 2238 0 ARG 1718 36.201 -0.623 7.428 1.00 30.60 ATOM 2239 N MET 1719 34.056 -0.430 8.074 1.00 30.69 **ATOM** 2241 CA MET 1719 34.350 -0.490 9.501 1.00 31.77 **ATOM** 2242 CB MET 1719 33.072 -0.302 10.335 1.00 34.56 MOTA 2243 CG MET 1719 32.408 1.060 10.194 1.00 36.71 MOTA 2244 SD MET 1719 31.015 1.307 11.314 1.00 38.66 ATOM 2245 CE MET 1719 29.797 0.338 10.544 1.00 36.99 MOTA 2246 С MET 1719 34.998 -1.810 9.854 1.00 30.20 MOTA 2247 0 MET 1719 34.802 -2.802 9.169 1.00 31.41 MOTA 2248 N **ASP** 1720 35.778 10.926 -1.809 1.00 32.49 MOTA 2250 CA ASP 1720 36.473 -3.008 11.385 1.00 33.60 ATOM 2251 CB 1720 ASP 37.593 -2.630 12.358 1.00 37.65 ATOM 2252 CG ASP 1720 38.628 -1.688 11.747 1.00 44.69 ATOM 2253 50.97 OD1 **ASP** 1720 38.442 -1.223 10.596 1.00 MOTA 2254 OD2 ASP 1720 39.632 -1.398 12.443 1.00 48.67 MOTA 2255 C ASP 1720 35.524 -3.977 12.079 1.00 31.26 MOTA 2256 0 34.466 ASP 1720 -3.581 12.561 1.00 32.69 **ATOM** 2257 N LYS 1721 35.943 -5.231 12.191 1.00 32.76 MOTA 2259 CA LYS 1721 35.133 -6.261 12.825 1.00 32.28 **ATOM** 2260 CB LYS 1721 35.726 -7.649 12.575 1.00 33.63 MOTA 2261 CG LYS 1721 34.854 -8.773 13.125 1.00 35.68 ATOM 2262 CD LYS 1721 35.392 -10.126 12.784 1.00 36.22 MOTA 2263 CE LYS 1721 36.054 -10.749 13.988 1.00 42.65 MOTA 2264 NZ LYS 1721 36.354 -12.189 13.756 1.00 46.15 ATOM 2268 C LYS 1721 35.039 -6.051 1.00 14.315 35.55 **ATOM** 2269 36.064 0 LYS 1721 -5.926 14.986 1.00 37.78 MOTA 2270 N PRO 1722 33.807 -6.017 14.861 1.00 36.91 MOTA 2271 CD PRO 1722 32.504 -6.105 14.179 1.00 34.43 MOTA 2272 CA PRO 1722 33.630 -5.827 16.305 1.00 37.77 MOTA 2273 CB PRO 1722 32.107 -5.846 16.465 1.00 36.32 MOTA 2274 CG PRO 1722 31.603 -5.375 15.122 1.00 34.53 MOTA 2275 C PRO 1722 34.246 -7.026 17.023 1.00 39.31 MOTA 2276 0 PRO 1722 34.274 -8.136 16.477 1.00 38.78 **ATOM** 2277 N 1723 SER 34.777 -6.820 18.222 1.00 42.72 MOTA 2279 CA SER 1723 35.336 -7.954 18.940 1.00 45.01 MOTA 2280 CB SER 1723 36.152 -7.508 20.160 1.00 46.88 MOTA 2281 OG 1723 SER 35.327 -7.027 21.208 1.00 53.47 MOTA 2283 C SER 1723 34.088 -8.731 19.359 1.00 46.67 MOTA 2284 0 SER 1723 32.982 -8.172 19.417 1.00 46.21 MOTA 2285 N ASN 1724 34.237 -10.025 19.590 1.00 47.80 MOTA 2287 CA ASN 1724 33.092 -10.826 19.999 1.00 52.78 MOTA 2288 СВ ASN 1724 32.559 -10.319 21.355 1.00 57.86 MOTA 2289 CG ASN 1724 33.679 -10.091 22.370 1.00 61.99 ATOM 2290 OD1 ASN 1724 34.531 -10.959 22.585 1.00 63.17 MOTA 2291 ND2 ASN 1724 33.712 -8.899 22.953 1.00 63.56 MOTA 2294 С ASN 1724 32.015 -10.779 18.893 1.00 51.43 MOTA 2295 0 ASN 1724 30.859 -10.423 19.108 1.00 51.56 **ATOM** 2296 N CYS 1725 32.454 -11.087 17.683 1.00 48.91 ATOM 2298 1725 CA CYS 31.600 -11.136 16.508 1.00 45.62 MOTA 2299 CB CYS 1725 31.526 -9.771 15.811 1.00 44.83 **ATOM** 2300 SG 1725 CYS 30.693 -9.816 14.194 1.00 41.83 MOTA 2301 С CYS 1725 32.341 -12.135 15.640 1.00 42.30

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ATOM 2302 o **CYS** 1725 33.566 -12.045 15.493 1.00 44.63 ATOM 2303 N THR 1726 31.627 -13.134 15.141 1.00 37.46 ATOM 2305 CA THR 1726 32.259 -14.153 14.320 1.00 35.29 **ATOM** 2306 CB THR 1726 31.339 -15.367 1.00 14.132 33.44 **ATOM** 2307 OG1 THR 1726 30.109 -14.952 13.523 1.00 34.77 MOTA 2309 CG2 THR 1726 31.070 -16.019 15.454 1.00 30.22 2310 MOTA C THR 1726 32.668 -13.622 12.963 1.00 33.53 MOTA 2311 0 THR 1726 32.158 -12.593 12.518 1.00 32.93 MOTA 2312 N ASN 1727 33.619 -14.294 12.319 1.00 32.72 MOTA 2314 CA ASN 1727 34.030 -13.867 10.983 1.00 35.91 MOTA 2315 CB ASN 1727 35.166 -14.724 10.422 1.00 40.64 **ATOM** 2316 CG ASN 1727 36.463 -14.533 11.168 1.00 46.52 MOTA 2317 OD1 ASN 1727 37.047 -13.453 11.158 1.00 49.98 MOTA 2318 ND2 ASN 1727 ..11.814 36.931 -15.592 1.00 49.04 MOTA 2321 C ASN 1727 32.824 -14.006 10.058 1.00 34.27 MOTA 2322 0 ASN 1727 32.681 -13.236 9.116 1.00 32.96 **MOTA** 2323 N GLU 1728 31.969 -14.997 10.326 1.00 32.49 **ATOM** 2325 CA GLU 1728 30.778 -15.235 9.510 1.00 31.99 2326 **ATOM** CB GLU 1728 30.064 -16.504 9.975 1.00 34.15 **ATOM** 2327 CG GLU 1728 28.836 -16.866 9.156 1.00 35.63 **ATOM** 2328 CD GLU 1728 28.187 -18.169 9.608 1.00 39.72 **ATOM** 2329 OE1 GLU 1728 28.200 -18.463 10.824 1.00 42.25 MOTA 2330 OE2 GLU 1728 27.654 -18.896 8.742 1.00 39.87 MOTA 2331 C GLU 1728 -14.049 29.814 9.549 1.00 30.76 MOTA 2332 0 GLU 1728 29.309 -13.602 8.512 1.00 29.58 **ATOM** 2333 N LEU 1729 29.559 -13.544 10.750 1.00 30.01 **ATOM** 2335 CA LEU 1729 28.670 -12.408 10.911 1.00 30.21 **ATOM** 2336 CB LEU 1729 28.225 -12.272 12.364 1.00 30.13 **ATOM** 2337 CG LEU 1729 27.208 -13.350 12.748 1.00 33.61 **ATOM** 2338 CD1 LEU 1729 27.119 -13.483 14.262 1.00 33.71 ATOM 2339 CD2 LEU 1729 25.844 -13.021 12.139 1.00 30.31 MOTA 2340 C LEU 1729 29.316 -11.133 10.390 1.00 30.26 MOTA 2341 0 LEU 1729 28.619 -10.229 9.938 1.00 28.89 MOTA 2342 N TYR 1730 30.648 -11.063 10.435 1.00 28.91 MOTA 2344 CA TYR 1730 31.343 -9.893 9.912 1.00 28.91 MOTA 2345 CB TYR 1730 32.804 -9.861 10.359 1.00 29.09 MOTA 2346 CG TYR 1730 33.537 -8.639 9.857 1.00 30.15 MOTA 2347 CD1 TYR 1730 33.037 -7.358 10.103 1.00 29.97 MOTA 2348 CEL TYR 1730 33.688 -6.227 9.626 1.00 28.99 MOTA 2349 CD2 TYR 1730 34.716 -8.757 9.119 1.00 29.24 MOTA 2350 CE2 TYR 1730 35.386 -7.620 8.632 1.00 28.25 MOTA 2351 CZ TYR 1730 34.861 ~6.362 8.889 1.00 28.41 ATOM 2352 OH TYR 1730 35.485 -5.227 8.405 1.00 31.64 MOTA 2354 С TYR 1730 31.260 -9.943 8.379 1.00 27.10 **ATOM** 2355 0 TYR 1730 31.078 -8.920 7.726 1.00 27.46 MOTA 2356 N MET 1731 31.390 -11.138 7.813 1.00 26.68 MOTA 2358 CA MET 1731 31.298 28.68 -11.315 6.372 1.00 2359 ATOM CB MET 1731 31.526 -12.778 5.989 1.00 35.43 MOTA 2360 CG MET 1731 31.158 -13.087 4.545 1.00 46.19 MOTA 2361 SD MET 1731 31.441 -14.804 4.064 1.00 60.10 MOTA 2362 CE MET 1731 32.603 -14.550 2.678 1.00 58.31 MOTA 2363 C MET 1731 29.917 -10.858 5.912 1.00 27.42 MOTA 2364 0 MET 1731 29.782 -10.227 4.871 1.00 30.80 MOTA 2365 N MET 1732 28.893 -11.191 6.688 1.00 28.53

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MOTA 2367 CA MET 1732 27.522 -10.777 6.389 1.00 26.47 MOTA 2368 CB MET 1732 26.562 -11.308 7.458 1.00 25.79 **ATOM** 2369 CG MET 1732 25.116 -10.838 7.274 1.00 26.01 MOTA 2370 SD MET 1732 24.004 -11.550 8.469 1.00 26.22 MOTA 2371 CE MET 1732 23.787 -13.195 7.783 1.00 23.74 ATOM 2372 C MET 1732 27.445 -9.243 6.319 1.00 25.15 ATOM 2373 0 MET 1732 26.886 -8.691 5.379 1.00 25.41 ATOM 2374 N MET 1733 28.024 -8.564 7.308 1.00 26.48 MOTA 2376 CA MET 1733 28.057 -7.104 7.331 1.00 27.09 **ATOM** 1.00 2377 CB MET 1733 28.903 ~6.594 8.488 25.91 MOTA 2378 CG MET 1733 28.235 -6.556 9.824 1.00 31.64 MOTA 2379 SD MET 1733 29.442 -6.111 11.094 1.00 29.59 MOTA 2380 CE MET 1733 28.886 -7.126 12.420 1.00 28.14 2381 MOTA С MET 1733 28.720 -6.613 6.056 1.00 28.43 ATOM 2382 0 MET 1733 28.185 -5.753 5.372 1.00 31.37 MOTA 2383 N ARG 1734 29.891 -7.169 5.747 1.00 28.57 MOTA 2385 CA ARG 1734 30.642 -6.783 4.551 1.00 27.00 MOTA 2386 CB ARG 1734 32.007 -7.488 4.510 1.00 25.98 MOTA 2387 CG ARG 1734 32.927 -7.154 5.707 1.00 28.13 MOTA 2388 CD ARG 1734 33.229 -5.672 5.765 1.00 29.97 MOTA 2389 NE ARG 1734 33.922 -5.256 4.553 1.00 40.49 MOTA 2391 CZARG 1734 35.238 -5.361 4.363 1.00 43.95 MOTA 2392 NH1 ARG 1734 36.023 -5.853 5.318 1.00 41.81 MOTA 2395 NH2 ARG 1734 35.760 -5.048 3.184 1.00 46.20 MOTA 2398 С ARG 1734 29.859 -7.037 3.268 1.00 24.57 MOTA 2399 -6.290 0 ARG 1734 29.992 24.94 2.314 1.00 MOTA 2400 N ASP 1735 29.071 -8.107 3.235 1.00 24.79 MOTA 2402 ASP 1735 CA 28.254 -8.420 2.061 1.00 23.88 MOTA 2403 CB ASP 1735 27.669 -9.830 2.150 1.00 25.95 MOTA 2404 ASP CG 1735 28.724 -10.913 2.024 1.00 27.60 **ATOM** 2405 OD1 **ASP** 1735 29.842 -10.632 1.529 1.00 27.75 MOTA 2406 OD2 ASP 1735 28.432 -12.051 2.430 1.00 28.90 MOTA 2407 С ASP 1735 1.00 27.139 -7.396 1.941 22.61 MOTA 2408 ASP 1735 0 26.777 -6.996 0.833 1.00 22.66 **ATOM** 2409 N CYS 1736 26.611 -6.965 3.085 1.00 20.61 MOTA 2411 CA CYS 1736 25.561 -5.952 3.109 1.00 23.63 ATOM 2412 CB CYS 1736 25.007 -5.767 4.534 1.00 21.98 MOTA 2413 1736 SG CYS 23.934 -7.126 5.111 1.00 22.95 MOTA 2414 С CYS 1736 26.129 -4.633 2.599 1.00 23.62 MOTA 2415 0 CYS 1736 25.403 -3.797 22.15 2.047 1.00 MOTA 2416 N TRP 1737 27.438 -4.461 2.775 1.00 24.37 MOTA 2418 CA TRP 1737 28.123 -3.247 2.342 1.00 23.77 MOTA 2419 CB TRP 1737 29.162 -2.810 3.371 1.00 19.38 MOTA 2420 CG TRP 1737 28.601 -2.520 4.718 1.00 21.62 **ATOM** 2421 CD2 TRP 1737 29.268 -2.688 5.971 1.00 24.81 MOTA 2422 CE2 TRP 1737 28.371 -2.278 6.980 1.00 25.95 ATOM 2423 CE3 TRP 1737 30.534 -3.165 6.340 1.00 29.02 **MOTA** 2424 CD1 TRP 1737 27.359 -2.024 5.007 1.00 23.21 **ATOM** 2425 NE1 TRP 1737 27.213 -1.876 6.362 1.00 21.80 ATOM 2427 CZ2 TRP 1737 28.710 -2.305 8.347 1.00 26.68 MOTA 2428 CZ3 TRP 1737 30.873 -3.198 7.699 1.00 31.06 **ATOM** 2429 CH2 TRP 1737 29.959 -2.774 8.685 1.00 30.18 MOTA 2430 C TRP 1737 28.788 -3.372 0.978 1.00 24.88 ATOM 2431 O TRP 1737 29.737 -2.646 0.689 1.00 25.11

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MOTA	2432	N	HIS	1738	28.303	-4.278	0.132	1.00	25.27
ATOM	2434	CA	HIS	1738	28.888	-4.406	-1.191	1.00	24.27
ATOM	2435	CB	HIS	1738	28.280	-5.573	-1.986	1.00	25.24
MOTA	2436	CG	HIS	1738	29.179	-6.073	-3.081	1.00	26.28
ATOM	2437	CD2	HIS	1738	29.727	-5.437	-4.147	1.00	25.67
ATOM	2438	ND1	HIS	1738	29.697	-7.352	-3.098	1.00	27.55
MOTA	2440	CE1	HIS	1738	30.528	-7.478	-4.117	1.00	27.51
MOTA	2441	NE2	HIS	1738	30.564	-6.329	-4.770	1.00	30.93
ATOM	2443	C	HIS	1738	28.715	-3.087	-1.953	1.00	25.59
ATOM	2444	0	HIS	1738	27.659	~2.451	-1.905	1.00	22.01
MOTA	2445	N	ALA	1739	29.784	-2.651	-2.612	1.00	23.84
ATOM	2447	CA	ALA	1739	29.759	-1.418	-3.388	1.00	24.93
ATOM	2448	СВ	ALA	1739	31.131	-1.177	-4.024	1.00	26.39
ATOM	2449	С	ALA	1739	28.671	-1.508	-4.462	1.00	25:35
MOTA	2450	0	ALA	1739	27.963	-0.535	-4.727	1.00	28.20
MOTA	2451	N	VAL	1740	28.543	-2.680	-5.073	1.00	22.68
ATOM	2453	CA	VAL	1740	27.528	-2.904	-6.101	1.00	26.46
ATOM	2454	СВ	VAL	1740	27.995	-3.968	-7.117	1.00	29.70
ATOM	2455	CG1	VAL	1740	27.063	-4.003	-8.334	1.00	26.01
ATOM	2456	CG2	VAL	1740	29.433	-3.686	-7.537	1.00	31.22
MOTA	2457	С	VAL	1740	26.213	-3.358	-5.443	1.00	25.07
MOTA	2458	0	VAL	1740	26.138	-4.474	-4.903	1.00	23.55
ATOM	2459	N	PRO	1741	25.155	-2.519	-5.514	1.00	25.30
MOTA	2460	CD	PRO	1741	25.133	-1.190	-6.153	1.00	22.43
ATOM	2461	CA	PRO	1741	23.844	-2.833	-4.921	1.00	24.09
MOTA	2462	CB	PRO	1741	22.962	-1.675	-5.402	1.00	23.12
ATOM	2463	CG	PRO	1741	23.928	-0.527	-5.491	1.00	22.04
ATOM	2464	С	PRO	1741	23.272	-4.191	-5.313	1.00	22.18
ATOM	2465	0	PRO	1741	22.727	-4.900	-4.466	1.00	21.23
MOTA	2466	N	SER	1742	23.437	-4.570	-6.580	1.00	23.87
ATOM	2468	CA	SER	1742	22.928	-5.847	-7.088	1.00	24.36
MOTA	2469	CB	SER	1742	23.071	-5.907	-8.612	1.00	27.39
MOTA	2470	OG	SER	1742	24.436	-6.025	-8.986	1.00	29.25
ATOM	2472	С	SER	1742	23.636	-7.058	-6.488	1.00	23.96
MOTA	2473	0	SER	1742	23.145	-8.179	-6.575	1.00	24.30
MOTA	2474	N	GLN	1743	24.810	-6.839	-5.915	1.00	24.39
ATOM	2476	CA	GLN	1743	25.558	-7.934	-5.345	1.00	23.15
ATOM	2477	CB	GLN	1743	27.046	-7.755	-5.638	1.00	23.83
ATOM	2478	CG	GLN	1743	27.359	-7.784	-7.126	1.00	22.84
ATOM	2479	CD	GLN	1743	26.816	-9.036	-7.808	1.00	24.20
ATOM	2480	OE1	GLN	1743	27.318	-10.135	-7.590	1.00	21.50
ATOM	2481	NE2	GLN	1743	25.775	-8.871	-8.628	1.00	22.45
ATOM	2484	С	GLN	1743	25.309	-8.171	-3.868	1.00	23.12
ATOM	2485	0	GLN	1743	25.816	-9.135	-3.317	1.00	24.96
ATOM	2486	N	ARG	1744	24.557	-7.280	-3.225	1.00	23.67
ATOM	2488	CA	ARG	1744	24.242	-7.424	-1.806	1.00	22.11
ATOM	2489	СВ	ARG	1744	23.699	-6.110	-1.231	1.00	19.70
ATOM	2490	CG	ARG	1744	24.672	-4.959	-1.338	1.00	21.26
ATOM	2491	CD	ARG	1744	24.049	-3.640	-0.890	1.00	20.68
MOTA	2492	NE	ARG	1744	24.923	-2.552	-1.305	1.00	25.21
MOTA	2494	CZ	ARG	1744	24.540	-1.313	-1.583	1.00	24.30
MOTA	2495	NH1	ARG	1744	23.257	-0.955	-1.481	1.00	22.04
ATOM	2498	NH2	ARG	1744	25.450	-0.448	-2.036	1.00	21.29
ATOM	2501	C	ARG	1744	23.184	-8.505	-1.640	1.00	22.53
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MOTA 2502 0 ARG 1744 22.437 -8.800 -2.588 1.00 23.08 2503 MOTA 1745 N PRO 23.162 -9.170 -0.467 1.00 20.76 MOTA 2504 CD PRO 1745 24.087 -9.078 0.681 1.00 21.71 ATOM 2505 CA PRO 1745 22.160 -10.207 -0.243 1.00 22.34 PRO MOTA 2506 CB 1745 22.632 -10.859 1.057 1.00 20.58 MOTA 2507 CG PRO 1745 23.298 -9.727 1.783 1.00 20.36 MOTA 2508 С PRO 1745 20.814 -9.512 -0.048 1.00 23.62 MOTA 2509 0 PRO 1745 20.759 -8.318 0.255 1.00 25.29 MOTA 2510 N THR 1746 19.731 -10.235 -0.275 1.00 23.39 MOTA 2512 CA THR 1746 18.404 -9.675 -0.080 1.00 22.77 СВ ATOM 2513 THR 1746 17.386 -10.368 -1.004 1.00 23.24 **ATOM** 2514 OG1 THR 1746 17.409 -11.783 -0.763 1.00 23.11 ATOM 2516 CG2 THR 1746 17.724 -10.103 -2.475 1.00 24.96 2517 C MOTA 1746 THR 18.009 -9.954 1.365 1.00 24.98 MOTA 2518 0 THR 1746 18.664 -10.758 2.043 1.00 24.30 MOTA 2519 N PHE 1747 16.944 ~9.318 1.853 1.00 24.95 MOTA 2521 CA PHE 1747 16.501 -9.596 3.221 1.00 25.16 MOTA 2522 CB PHE 1747 15.395 -8.628 3.661 1.00 23.64 MOTA 2523 CG PHE 1747 15.916 -7.283 4.089 1.00 24.34 MOTA 2524 CD1 PHE 1747 16.715 -7.167 5.226 1.00 21.21 MOTA 2525 CD2 PHE 1747 15.649 -6.137 3.334 1.00 21.42 ATOM 2526 CE1 PHE 1747 17.252 -5.932 5.597 1.00 20.99 MOTA 2527 CE₂ PHE 1747 16.178 -4.907 3.699 1.00 20.36 MOTA 2528 CZ PHE 1747 16.985 -4.807 4.840 1.00 19.30 MOTA 2529 C PHE 1747 16.034 -11.049 3.311 1.00 23.57 MOTA 2530 O PHE 1747 16.182 -11.702 4.344 1.00 25.32 2531 MOTA LYS N 1748 15.520 -11.573 2.202 1.00 23.19 MOTA 2533 CA LYS 1748 15.066 -12.958 2.167 1.00 23.67 MOTA 2534 CB LYS 1748 14.462 -13.285 0.799 1.00 26.67 MOTA 2535 CG LYS 1748 14.018 -14.739 0.622 1.00 30.49 MOTA 2536 CD LYS 1748 13.642 -14.996 -0.837 1.00 38.98 MOTA 2537 CE LYS 1748 13.182 -16.432 -1.087 1.00 44.52 MOTA 2538 NZ LYS 1748 11.997 -16.790 -0.245 1.00 52.75 MOTA 2542 1748 С LYS 16.264 -13.B65 2.445 1.00 25.65 ATOM 2543 LYS 0 1748 16.184 -14.778 3.270 1.00 27.19 ATOM 2544 N GLN 1749 17.378 -13.603 1.762 1.00 24.56 MOTA 2546 CA GLN 1749 18.588 -14.397 1.950 1.00 26.33 ATOM 2547 CB GLN 1749 19.702 -13.953 0.993 1.00 27.97 2548 MOTA CG GLN 1749 19.416 -14.066 -0.484 1.00 37.31 MOTA 2549 CD GLN 1749 20.518 -13.415 -1.315 1.00 40.24 MOTA 2550 OEl GLN 1749 20.296 -12.408 -1.970 1.00 38.83 MOTA 2551 NE2 GLN 1749 21.726 -13.983 -1.259 1.00 47.83 MOTA 2554 GLN С 1749 19.099 -14.223 3.377 1.00 23.92 ATOM 2555 0 GLN 1749 19.459 -15.196 4.040 1.00 25.27 ATOM 2556 N LEU 1750 19.155 -12.976 3.829 1.00 23.12 MOTA 2558 CA LEU 1750 19.641 -12.662 5.175 1.00 24.34 MOTA 2559 CB LEU 1750 19.607 -11.149 5.427 1.00 23.08 **MOTA** 2560 CG LEU 1750 20.633 -10.311 4.665 1.00 23.84 MOTA 2561 CD1 LEU 1750 20.274 -8.806 4.724 1.00 22.10 **ATOM** 2562 CD2 LEU 1750 22.013 -10.586 24.91 5.246 1.00 MOTA 2563 С LEU 1750 18.840 -13.400 6.236 1.00 27.40 **MOTA** 2564 0 LEU 1750 19.408 -13.915 7.211 1.00 27.11 MOTA 2565 N VAL 1751 17.527 -13.482 6.031 1.00 26.83 MOTA 2567 16.665 CA VAL 1751 -14.174 6.970 1.00 25.31

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MOTA 2568 CB VAL 1751 15.176 -13.994 6.599 1.00 25.87 MOTA 2569 CG1 VAL 1751 14.304 -14.975 7.382 1.00 28.43 ATOM 2570 CG2 VAL 1751 14.746 -12.593 6.934 1.00 21.52 MOTA 2571 C VAL 1751 17.047 -15.642 7.025 1.00 25.87 MOTA 2572 O VAL 1751 17.178 -16.218 8.106 1.00 23.41 **ATOM** 2573 N GLU 1752 17.253 -16.243 5.858 1.00 29.98 MOTA 2575 CA GLU 1752 17.631 -17.651 5.799 1.00 33.12 MOTA 2576 CB GLU 1752 17.653 -18.134 4.346 1.00 35.99 MOTA 2577 CG GLU 1752 16.284 -18.077 3.670 1.00 43.58 MOTA 2578 CD GLU 1752 16.300 -18.5752.230 1.00 48.64 MOTA 2579 OE1 GLU 1752 15.453 -18.124 1.431 1.00 48.99 ATOM 2580 OE2 GLU 1752 17.157 -19.426 1.902 1.00 55.41 MOTA 2581: С GLU 1752 18.995 -17.891 6.467 1.00 33.15 ATOM 2582 O GLU .1752 .19.173 -18.847 7.236 1.00 30.71 **ATOM** 2583 N ASP 1753 19.951 -17.011 6.186 1.00 31.12 **ATOM** 2585 CA **ASP** 1753 21.279 ~17.131 6.770 1.00 30.51 **ATOM** 2586 CB **ASP** .1753 22.243 -16.108 6.155 1.00 29.15 ATOM 2587 CG **ASP** 1753 22.488 -16.344 4.672 1.00 33.53 MOTA 2588 OD1 ASP 1753 22.361 -17.494 4.215 1.00 34.92 MOTA 2589 OD2 **ASP** 1753 22.815 -15.371 3.955 1.00 38.26 **ATOM** 2590 C ASP 1753 21.215 -16.968 8.287 1.00 28.54 MOTA 2591 0 **ASP** 1753 21.739 -17.800 9.025 1.00 28.95 . ATOM 2592 N LEU 1754 20.537 -15.926 **B.753** 1.00 27.25 MOTA 2594 CA LEU 1754 20.421 -15.673 10.193 1.00 28.08 ATOM 2595 CB LEU 1754 19.754 -14.328 10.455 1.00 23.31 MOTA 2596 CG LEU 1754 20.733 -13.199 10.160 1.00 24.47 ATOM 2597 LEU CD1 1754 20.007 -11.863 10.094 1.00 19.58 MOTA 2598 LEU CD₂ 1754 21.846 -13.207 11.216 1.00 21.17 MOTA 2599 C LEU 1754 19.688 -16.789 10.921 1.00 31.61 MOTA 2600 0 LEU 1754 20.037 -17.135 12.048 1.00 32.64 MOTA 2601 N ASP 1755 18.690 -17.367 10.259 1.00 32.61 MOTA 2603 CA ASP 1755 17.931 -18.460 10.833 1.00 34.20 MOTA 2604 CB ASP 1755 16.823 -18.883 9.872 1.00 37.70 MOTA 2605 CG ASP 1755 15.808 -19.780 10.526 1.00 44.27 MOTA 2606 OD1 **ASP** 1755 15.445 -19.521 11.692 1.00 47.16 MOTA 2607 OD2 ASP 1755 15.370 -20.745 9.876 1.00 51.35 ATOM 2608 C ASP 1755 18.894 -19.616 11.073 1.00 34.63 MOTA 2609 0 ASP 1755 18.858 -20.273 12.119 1.00 36.24 MOTA 2610 N ARG 1756 19.782 -19.826 10.108 1.00 32.60 MOTA 2612 CA ARG 1756 20.784 -20.870 10.190 1.00 33.69 MOTA 2613 CB ARG 1756 21.548 -20.939 8.867 1.00 35.42 MOTA 2614 CG ARG 1756 22.639 -22.003 8.800 1.00 40.87 MOTA 2615 CD ARG 1756 23.212 -22.094 7.395 1.00 42.73 MOTA 2616 NE ARG 1756 23.739 -20.813 6.926 1.00 48.45 **ATOM** 2618 CZARG 1756 24.882 -20.274 7.340 1.00 49.90 MOTA 2619 NH1 ARG 1756 25.634 -20.905 8.243 1.00 49.63 MOTA 2622 NH2 ARG 1756 25.276 -19.105 6.844 1.00 50.86 **ATOM** 2625 C ARG 1756 21.748 -20.598 11.345 1.00 34.78 2626 **ATOM** 0 **ARG** 1756 21.929 -21.436 12.228 1.00 36.24 MOTA 2627 N ILE 1757 22.325 -19.402 11.363 1.00 35.35 MOTA 2629 CA ILE 1757 23.281 -19.018 12.392 1.00 35.54 **ATOM** 2630 CB ILE 1757 23.905 -17.631 12.103 1.00 34.99 **ATOM** 2631 CG₂ ILE 1757 24.955 -17.303 13.159 1.00 32.06 **MOTA** 2632 CG1 ILE 1757 24.547 1.00 -17.626 10.711 33.77

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MOTA 2633 CD1 ILE 1757 24.908 -16.247 10.185 1.00 31.44 MOTA 2634 C ILE 1757 22.698 -19.036 13.803 1.00 36.49 **ATOM** 2635 0 ILE 1757 23.337 -19.548 14.716 1.00 36.40 VAL MOTA 2636 N 1758 21.487 -18.515 13.988 1.00 36.91 MOTA 2638 CA VAL 1758 15.322 1.00 20.881 -18.498 38.68 MOTA -17.962 2639 CB VAL 1758 19.425 15.312 1.00 37.77 MOTA 2640 CG1 18.806 VAL 1758 -18.059 16.708 1.00 38.39 MOTA 2641 CG2 VAL 1758 19.392 -16.524 14.854 1.00 36.69 MOTA 2642 VAL 20.891 C 1758 -19.908 15.895 1.00 41.38 MOTA 2643 0 VAL 21.405 1758 -20.138 16.997 1.00 42.41 ALA MOTA 2644 N 1759 20.379 -20.851 15.111 1.00 40.59 MOTA 2646 CA ALA 1759 20.325 -22.247 15.508 1.00 40.84 MOTA 2647 CB ALA 1759 19.741 -23.074 14.384 1.00 40.20 MOTA 2648 C ALA 1759 21.703 -22.787 15.897 1.00 42.52 MOTA 2649 O ALA 1759 21.822 -23.594 16.809 1.00 44.78 MOTA 2650 N LEU 1760 22.740 -22.339 15.208 1.00 43.16 MOTA 2652 CA LEU 1760 24.095 -22.800 15.493 1.00 46.98 MOTA 2653 CB LEU 1760 24.921 -22.761 14.203 1.00 47.66 MOTA 2654 CG LEU 1760 24.286 -23.545 13.060 1.00 52.77 MOTA 2655 CD1 LEU 1760 24.973 -23.222 11.745 1.00 56.58 MOTA 2656 CD₂ LEU 1760 24.343 -25.038 13.369 1.00 53.06 MOTA 2657 C LEU 1760 24.811 -21.986 16.573 1.00 47.43 **ATOM** 2658 O LEU 1760 25.917 -22.335 16.989 1.00 46.58 **ATOM** 2659 N THR 1761 24.183 -20.914 17.034 1.00 48.65 **ATOM** 2661 CA THR 1761 24.814 -20.055 18.021 1.00 49.69 MOTA 2662 CB THR 1761 24.382 -18.570 17.831 1.00 50.15 **MOTA** 2663 OG1 THR 1761 24.783 -18.127 16.529 1.00 49.87 **ATOM** 2665 CG2 THR 1761 25.063 -17.671 18.843 1.00 48.64 MOTA 2666 С THR 1761 24.673 -20.497 19.475 1.00 50.33 MOTA 2667 0 THR 1761 23.584 -20.825 19.947 1.00 48.81 MOTA 2668 N SER 1762 25.811 -20.511 20.166 1.00 50.25 MOTA 2670 CA SER 1762 25.891 -20.890 21.566 1.00 50.98 ATOM 2671 CB SER 1762 27.362 -20.887 22.002 1.00 54.71 MOTA 2672 OG SER 1762 27.537 -21.423 23.308 1.00 57.99 MOTA 2674 С SER 1762 25.083 -19.914 22.425 1.00 49.39 MOTA 2675 О SER 1762 25.297 -18.694 22.370 1.00 48.00 MOTA 3474 N SER 461 79.623 25.766 14.533 1.00 48.84 MOTA 3476 CA SER 461 79.566 24.645 13.593 1.00 46.93 ATOM 3477 SER CB 461 78.276 23.838 13.809 1.00 46.66 ATOM 3478 C SER 461 79.676 25.114 43.02 12.138 1.00 ATOM 3479 0 SER 461 79.692 24.301 11.210 1.00 40.19 ATOM 3480 N GLU 462 79.791 26.427 11.956 1.00 41.48 MOTA 3482 CA GLU 462 79.904 27.034 10.628 1.00 39.59 MOTA 3483 CB GLU 462 80.021 28.560 10.744 1.00 40.66 ATOM 3484 С GLU 462 81.054 26.480 9.796 1.00 36.60 MOTA 3485 0 GLU 462 80.852 26.121 8.641 1.00 35.10 MOTA 3486 N TYR 463 82.252 26.416 10.380 1.00 36.07 MOTA 3488 CA TYR 463 83.430 25.916 9.673 1.00 35.60 MOTA 3489 CB TYR 463 84.597 26.906 9.755 1.00 38.15 ATOM 3490 CG TYR 463 84.372 28.104 8.861 1.00 44.08 MOTA 3491 CD1 TYR 463 84.137 29.368 9.406 1.00 44.99 **ATOM** 3492 CE1 TYR 463 83.833 30.451 8.593 1.00 46.88 MOTA 3493 CD2 TYR 463 84.305 27.959 7.464 1.00 43.95 ATOM 3494 TYR CE2 463 84.003 29.044 6.642 1.00 41.86

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ATOM	3495	CZ	TYR	463	83.768	30.282	7.215	1.00	43.89
ATOM	3496	OH	TYR	463	83.468	31.364	6.431	1.00	44.37
ATOM	3498	С	TYR	463	83.903	24.520	10.014	1.00	33.90
ATOM	3499	0	TYR	463	84.440	23.828	9.147	1.00	33.90
ATOM	3500	N	GLU	464	83.742	24.098	11.260	1.00	32.81
ATOM	3502	CA	GLU	464	84.167	22.753	11.633	1.00	34.64
MOTA	3503	CB	GLU	464	85.663	22.727	11.919	1.00	37.48
MOTA	3504	CG	GLU	464	86.075	23.633	13.049	1.00	45.48
ATOM	3505	CD	GLU	464	87.552	23.987	13.015	1.00	55.80
MOTA	3506	OE1	GLU	464	87.920	24.996	13.659	1.00	61.78
MOTA	3507	OE2	GLU	464	88.344	23.271	12.351	1.00	58.34
MOTA	3508	С	GLU	464	83.426	22.296	12.858	1.00	33.05
MOTA	3509	0	GLU	464	83:083	23.119	13.705	1.00	34.54
MOTA	3510	N	LEU	465	83.147	21.001	12.943	1:00	32.59
MOTA	3512	CA	LEU	465	82.462	20.463	14.114	1.00	33.74
ATOM	3513	CB	LEU	465	81.484	19.341	13.747	1.00	31.20
ATOM	3514	CG	LEU	465	80.510	19.433	12.577	1.00	32.77
MOTA	3515	CD1	LEU	465	79.355	18.492	12.858	1.00	26.22
MOTA	3516	CD2	LEU	465	80.021	20.846	12.359	1.00	31.59
ATOM	3517	С	LEU	465	83.511	19.889	15.059	1.00	35.64
ATOM	3518	0	LEU	465	84.641	19.574	14.642	1.00	33.77
MOTA	3519	N	PRO	466	83.150	19.734	16.349	1.00	36.71
ATOM	3520	CD	PRO	466	81.865	20.104	16.967	1.00	36.97
ATOM	3521	CA	PRO	466	84.074	19.185	17.346	1.00	36.17
MOTA	3522	CB	PRO	466	83.247	19.196	18.626	1.00	36.83
ATOM	3523	CG	PRO	466	82.274	20.326	18.394	1.00	40.80
ATOM	3524	С	PRO	466	84.419	17.765	16.950	1.00	37.39
MOTA	3525	0	PRO	466	83.626	17.077	16.297	1.00	34.71
ATOM	3526	N	GLU	467	85.611	17.330	17.315	1.00	38.40
MOTA	3528	CA	GLU	467	86.030	15.987	16.976	1.00	42.59
MOTA	3529	CB	GLU	467	87.493	15.987	16.540	1.00	49.21
ATOM	3530	CG	GLU	467	87.922	14.682	15.891	1.00	58.93
MOTA	3531	CD	GLU	467	89.276	14.769	15.213	1.00	64.76
MOTA	3532	OE1	GLU	467	90.013	15.767	15.426	1.00	63.57
MOTA	3533	OE2	GLU	467	B9.592	13.823	14.458	1.00	69.03
MOTA	3534	С	GLU	467	B5.82 5	15.037	18.146	1.00	40.74
MOTA	3535	0	GLU	467	85.938	15.430	19.309	1.00	41.52
MOTA	3536	N	ASP	468	85.472	13.802	17.831	1.00	38.57
ATOM	3538	CA	ASP	468	85.273	12.776	18.851	1.00	40.86
ATOM	3539	CB	ASP	468	83.793	12.640	19.224	1.00	40.27
MOTA	3540	CG	ASP	468	83.566	11.697	20.397	1.00	41.36
MOTA	3541	OD1	ASP	468	82.429	11.670	20.919	1.00	42.50
ATOM	3542	OD2	ASP	468	84.514	10.992	20.807	1.00	38.55
MOTA	3543	C	ASP	468	85.803	11.470	18.278	1.00	40.75
MOTA	3544	0	ASP	468	85.068	10.701	17.650	1.00	41.80
MOTA	3545	N	PRO	469	87.100	11.209	18.481	1.00	41.71
MOTA	3546	CD	PRO	469	88.001	12.062	19.276	1.00	41.87
MOTA	3547	CA	PRO	469	87.801	10.011	18.012	1.00	40.07
MOTA	3548	CB	PRO	469	89.091	10.042	18.831	1.00	40.42
ATOM	3549	CG	PRO	469	89.366	11.505	18.938	1.00	39.42
MOTA	3550	C	PRO	469	87.033	8.720	18.260	1.00	41.00
MOTA	3551	0	PRO	469	87.032	7.822	17.414	1.00	41.75
MOTA	3552	N	ARG	470	86.361	8.639	19.411	1.00	40.70
ATOM	3554	CA	ARG	470	85.600	7.446	19.779	1.00	41.03
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MOTA 3555 ARG 470 CB 84.827 7.677 21.075 1.00 44.18 MOTA 3556 CG ARG 470 85.628 8.240 22.218 1.00 47.89 MOTA 3557 CD ARG 470 84.719 8.518 23.400 1.00 50.56 MOTA 3558 NE ARG 470 83.576 9.345 23.023 1.00 51.20 MOTA 3560 CZ ARG 470 82.695 9.845 23.881 1.00 52.24 MOTA 3561 NH1 ARG 470 82.818 9.608 25.183 1.00 51.31 MOTA 3564 NH2 ARG 470 81.672 10.564 23.432 1.00 52.73 MOTA 3567 С ARG 470 84.596 7.004 18.723 1.00 39.03 MOTA 3568 0 ARG 470 84.401 5.813 18.518 1.00 40.72 MOTA 3569 N TRP 471 83.972 7.965 18.050 1.00 37.77 MOTA 3571 CA TRP 471 82.948 7.656 17.059 1.00 36.73 MOTA 3572 CB TRP 471 81.672 8.401 17.432 1.00 35.05 MOTA 3573 CG TRP 471 81.044 7.862 18.673 1.00 34.85 MOTA 3574 CD2 TRP 471 80.235 6.687 18.766 1.00 34.96 MOTA 3575 CE2 TRP 471 79.831 6.564 20.116 1.00 35.12 MOTA 3576 CE3 TRP 471 79.810 5.721 17.838 1.00 33.25 MOTA 3577 CD1 TRP 471 81.106 8.390 19.933 1.00 29.97 ATOM 3578 NE1 TRP 471 80.377 7.616 20.805 1.00 32.18 MOTA 3580 CZ2 TRP 471 79.017 5.512 20.560 1.00 33.98 ATOM 3581 CZ3 TRP 471 79.002 4.673 18.282 1.00 33.71 ATOM 3582 CH2 TRP 471 78.618 4.580 19.632 1.00 33.28 MOTA 3583 C TRP 471 83.275 7.930 15.599 1.00 37.27 ATOM 3584 O TRP 471 82.580 7.445 14.695 1.00 36.61 MOTA 8.680 3585 N GLU 472 84.341 15.361 1.00 37.93 MOTA 3587 CA GLU 472 84.706 9.054 14.004 1.00 37.08 3588 ATOM CB GLU 472 85.865 10.049 14.045 1.00 36.30 MOTA 3589 CG GLU 472 86.026 10.851 12.773 1.00 33.51 MOTA 3590 CDGLU 472 84.931 11.895 12.580 1.00 33.80 MOTA 3591 GLU OE1 472 84.385 12.408 13.581 1.00 35.19 MOTA 3592 OE2 GLU 472 84.641 12.226 11.412 1.00 32.51 **ATOM** 3593 C GLU 472 85.021 7.923 13.032 1.00 37.88 MOTA 3594 0 GLU 472 85.774 7.000 13.351 1.00 38.20 MOTA 3595 N LEU 473 84.422 7.992 11.846 1.00 37.55 MOTA 3597 CA LEU 473 84.678 7.004 10.813 1.00 36.93 ATOM 3598 CB LEU 473 83.404 6.244 10.443 1.00 37.08 MOTA 3599 LEU CG 473 83.680 5.086 9.470 1.00 39.14 MOTA 3600 CD1 LEU 473 84.196 3.877 10.250 1.00 38.39 MOTA 3601 CD2 LEU 473 82.433 4.716 8.672 1.00 39.46 MOTA 3602 LEU 473 C 85.207 7.732 9.577 1.00 38.52 MOTA 3603 О LEU 473 84.660 8.764 9.182 1.00 38.67 MOTA 3604 N PRO 474 86.334 7.259 9.005 39.02 1.00 MOTA 3605 CD PRO 474 87.259 6.259 9.571 1.00 38.39 MOTA 3606 CA PRO 474 86.918 7.877 7.809 1.00 38.24 ATOM 3607 CB PRO 474 88.188 7.049 7.590 1.00 38.40 ATOM 3608 CG PRO 474 88.580 6.680 8.979 1.00 35.50 ATOM 3609 С PRO 474 85.942 7.727 6.642 1.00 37.56 MOTA 3610 0 PRO 474 85.415 6.641 6.400 1.00 37.88 MOTA 3611 85.720 ARG 475 N 8.809 5.907 1.00 37.73 ATOM 3613 CA ARG 475 84.779 8.790 4.795 1.00 40.01 ATOM 3614 CB ARG 475 84.655 10.183 4.182 1.00 38.31 **ATOM** 3615 84.217 CG ARG 475 11.236 5.198 1.00 35.15 **ATOM** 3616 CDARG 475 84.069 12.631 4.586 1.00 33.92 MOTA 475 3617 NE ARG 83.718 13.603 5.616 1.00 30.45 MOTA 3619 CZARG 475 82.475 13.880 5.993 1.00 26.48

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MOTA	3620	NH1	ARG	475	81.444	13.284	5.407	1.00	24.80
ATOM	3623	NH2	ARG	475	82.271	14.650	7.056	1.00	25.16
MOTA	3626	С	ARG	475	85.054	7.735	3.728	1.00	42.18
MOTA	3627	0	ARG	475	84.125	7.197	3.128	1.00	41.43
MOTA	3628	N	ASP	476	86.322	7.391	3.535	1.00	45.44
ATOM	3630	CA	ASP	476	86.676	6.387	2.541	1.00	49.80
MOTA	3631	CB	ASP	476	88.192	6.343	2.329	1.00	50.95
MOTA	3632	CG	ASP	476	88.944	5.975	3.585	1.00	53.89
MOTA	3633	OD1	ASP	476	89.303	4.789	3.731	1.00	59.71
ATOM	3634	OD2	ASP	476	89.176	6.867	4.427	1.00	57.39
ATOM	3635	С	ASP	476	86.149	5.010	2.950	1.00	51.23
ATOM	3636	0	ASP	476	86.051	4.102	2.121	1.00	53.54
MOTA	3637	N	ARG	477	85.814	4.864	4.230	1.00	50.49
ATOM	3639	CA		477	85.285	3.610	4.753	1.00	49.32
ATOM	3640	CB	ARG	477	85.834	3.364	6.152	1.00	49.79
MOTA	3641	CG	ARG	477	87.237	2.806	6.112	1.00	53.06
ATOM	3642	CD	ARG	477	87.960	2.981	7.420	1.00	56.76
MOTA	3643	NE	ARG	477	87.310	2.293	8.529	1.00	59.35
ATOM	3645	CZ	ARG	477	87.728	2.371	9.789	1.00	62.23
MOTA	3646	NH1	ARG	477	88.793	3.103	10.101	1.00	63.66
MOTA	3649	NH2	ARG	477	87.067	1.741	10.745	1.00	64.35
MOTA	3652	С	ARG	477	83.755	3.547	4.750	1.00	48.04
MOTA	3653	0	ARG	477	83.160	2.693	5.404	1.00	48.09
ATOM	3654	N	LEU	478	83.129	4.412	3.958	1.00	45.38
MOTA	3656	CA	LEU	478	81.685	4.469	3.870	1.00	41.60
MOTA	3657	CB	LEU	478	81.168	5.578	4.790	1.00	38.39
ATOM	3658	CG	LEU	478	79.651	5.699	4.894	1.00	36.38
MOTA	3659	CD1	LEU	478	79.113	4.595	5.802	1.00	33.98
MOTA	3660	CD2	LEU	478	79.293	7.068	5.441	1.00	40.06
MOTA	3661	С	LEU	478	81.279	4.774	2.433	1.00	41.92
ATOM	3662	0	LEU	478	81.696	5.780	1.870	1.00	43.99
MOTA	3663	N	VAL	479	80.466	3.904	1.844	1.00	42.29
MOTA	3665	CA	VAL	479	79.992	4.082	0.471	1.00	41.07
MOTA	3666	CB	VAL	479	80.227	2.816	-0.397	1.00	41.13
MOTA	3667	CG1	VAL	479	79.719	3.057	-1.810	1.00	40.19
MOTA	3668	CG2	VAL	479	81.700	2.448	-0.420	1.00	41.36
ATOM	3669	C	VAL	479	78.500	4.345	0.540	1.00	40.44
MOTA	3670	0	VAL	479	77.719	3.451	0.885	1.00	39.86
ATOM	3671	N	LEU	480	78.112	5.582	0.253	1.00	41.37
ATOM ATOM	3673	CA	LEU	480	76.706	5.973	0.293	1.00	41.63
	3674	CB	LEU	480	76.568	7.492	0.166	1.00	39.91
MOTA MOTA	3675	CG	LEU	480	77.236	8.332	1.261	1.00	39.23
	3676	CD1	LEU	480	76.890	9.800	1.039	1.00	37.73
ATOM	3677	CD2	LEU	480	76.791	7.877	2.647	1.00	35.18
ATOM	3678	С	LEU	480	75.899	5.273	-0.788	1.00	42.21
ATOM	3679	0	LEU	480	76.395	5.048	-1.890	1.00	45.27
ATOM ATOM	3680	N	GLY	481	74.650	4.947	-0.476	1.00	41.51
	3682	CA	GLY	481	73.812	4.257	-1.433	1.00	40.19
ATOM	3683	C	GLY	481	72.446	4.872	-1.640	1.00	41.58
ATOM	3684	0	GLY	481	72.262	6.091	-1.550	1.00	41.35
ATOM	3685	N	LYS	482	71.474	4.009	-1.908	1.00	42.65
ATOM	3687	CA	LYS	482	70.105	4.429	-2.166	1.00	44.17
ATOM	3688	CB	LYS	482	69.240	3.221	-2.542	1.00	45.66
MOTA	3689	С	LYS	482	69.475	5.148	-0.994	1.00	44.86

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ATOM 3690 Ο. LYS 482 69.638 1.00 4.752 0.155 45.23 **ATOM** 3691 PRO N 483 68.749 1.00 6.234 -1.273 45.94 **ATOM** 3692 CD PRO 483 68.518 6.880 -2.576 1.00 46.96 MOTA 3693 CA PRO 483 68.099 6.983 -0.206 1.00 47.79 MOTA 3694 CB PRO 483 67.542 8.200 -0.947 1.00 47.02 MOTA 3695 CG PRO 483 67.269 7.666 -2.307 1.00 46.65 MOTA 3696 C PRO 483 66.991 6.151 0.429 1.00 48.74 MOTA 3697 0 PRO 483 66.314 5.376 -0.251 1.00 48.01 ATOM 3698 N LEU 484 66.858 6.268 1.742 1.00 49.91 MOTA 3700 CA LEU 484 65.837 5.547 2.477 1.00 53.93 MOTA 3701 CB LEU 484 66.433 4.883 3.720 1.00 50.17 MOTA 3702 CG LEU 484 67.517 3.844 3.445 1.00 48.93 MOTA 3703 CD1 LEU 484 68.226 3.460 4.731 1.00 49.05 **ATOM** 3704 CD2 LEU 484 66.906 2.630 2.784 1.00 47.03 ATOM 3705 LEU C 484 64.715 6.501 2.878 1.00 58.70 ATOM 3706 0 LEU 484 63.571 6.075 3.055 1.00 61.95 ATOM 3707 N GLY 485 65.027 7.788 3.006 1.00 60.35 MOTA 3709 CA GLY 485 63.998 8.737 3.397 1.00 64.00 MOTA 3710 C GLY 485 64.445 10.183 3.476 1.00 66.09 MOTA 3711 0 GLY 485 65.643 10.468 3.577 1.00 65.26 **ATOM** 3712 N GLU 486 63.471 11.090 3.458 1.00 67.18 ATOM 3714 CA GLU 486 63.733 12.525 3.508 1.00 68.69 MOTA 3715 CB GLU 486 63.873 13.084 2.091 1.00 69.88 ATOM 3716 С GLU 486 62.618 13.249 4.245 1.00 68.80 MOTA 3717 0 GLU 486 61.481 12.775 4.295 1.00 69.26 MOTA 3718 N GLY 487 62.943 4.791 14.415 1.00 68.47 MOTA 3720 CA GLY 487 61.960 5.520 15.188 1.00 67.56 MOTA 3721 C GLY 487 62.373 16.635 5.634 1.00 66.71 MOTA 3722 0 GLY 487 63.040 17.172 4.747 1.00 66.48 MOTA 3723 N ALA 488 61.979 17.265 6.735 1.00 67.22 ATOM 3725 CA ALA 488 62.304 18.661 6.992 1.00 67.78 MOTA 3726 CB ALA 488 61.637 19.121 8.283 1.00 68.97 ATOM 3727 C ALA 488 63.817 18.830 7.085 1.00 67.38 MOTA 3728 0 ALA 488 64.413 18.597 1.00 8.141 67.14 MOTA 3729 N PHE 489 64.429 19.155 5.946 1.00 66.22 MOTA 3731 CA PHE 489 65.877 19.364 5.831 1.00 65.49 MOTA 3732 CB PHE 489 66.277 66.11 20.699 6.467 1.00 MOTA 3733 С PHE 66.749 489 18.207 6.368 1.00 64.07 MOTA 3734 0 PHE 489 67.924 18.399 6.731 1.00 61.56 MOTA 3735 N GLY 490 66.171 17.005 6.349 1.00 60.79 MOTA 3737 CA GLY 490 66.852 15.803 6.797 1.00 54.72 **ATOM** 3738 С GLY 490 66.787 14.760 5.692 1.00 51.78 MOTA 3739 65.765 0 GLY 490 14.624 5.013 1.00 49.17 MOTA 3740 N GLN 491 67.874 14.015 5.528 1.00 49.97 **MOTA** 3742 CA GLN 491 68.000 12.984 4.504 1.00 48.06 **ATOM** 3743 CB **GLN** 491 68.891 13.520 3.371 1.00 51.02 **ATOM** 3744 CG GLN 491 69.286 12.518 2.289 1.00 56.00 MOTA 3745 CD GLN 491 70.155 13.143 1.202 1.00 58.93 **MOTA** 3746 OE1 GLN 491 70.483 14.330 1.255 1.00 60.31 MOTA 3747 NE2 GLN 491 70.529 12.341 0.202 1.00 60.19 MOTA 3750 C GLN 491 68.623 11.720 5.114 1.00 45.59 MOTA 3751 0 GLN 491 69.511 11.792 5.959 1.00 45.22 MOTA 3752 N VAL 492 68.148 10.561 4.693 1.00 43.19 ATOM 3754 CA VAL 492 68.676 9.304 5.193 1.00 41.54

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MOTA 3755 CB VAL 492 67.655 8.584 6.087 1.00 41.74 3756 MOTA CG1 VAL 492 68.217 7.248 6.561 1.00 43.70 ATOM 3757 CG2 VAL 492 67.283 9.463 7.269 1.00 44.07 **ATOM** 3758 C VAL 492 68.971 3.993 8.424 1.00 39.72 **ATOM** 3759 0 VAL 492 68.125 3.108 8.271 1.00 39.81 **ATOM** 3760 N VAL 493 70.176 3.942 7.872 1.00 36.38 ATOM 3762 CA VAL 493 70.545 7.001 2.844 1.00 35.88 MOTA 3763 CB VAL 493 71.580 7.666 1.869 1.00 36.92 MOTA 3764 CG1 VAL 493 71.142 9.069 1.485 1.00 36.64 MOTA 3765 CG2 VAL 493 72.978 7.670 2.469 1.00 38.29 MOTA 3766 С VAL 493 71.131 5.689 3.351 1.00 36.03 3767 MOTA 0 VAL 493 71.693 5.617 4.443 1.00 36.57 MOTA 3768 N LEU 494 70.947 4.637 2.571 1.00 34.91 MOTA 3770 CA LEU 494 71.500 . 3.344 2.909 1.00 36.04 MOTA 3771 CB LEU 494 2.244 70.809 2.094 1.00 37.43 MOTA 3772 CG LEU 494 71.312 0.814 2.269 1.00 36.62 MOTA 3773 CD1 LEU 494 71.327 0.437 3.735 1.00 36.37 MOTA 3774 CD2 LEU 494 70.419 -0.118 1.479 1.00 40.70 ATOM 3775 C LEU 494 72.967 3.451 2.510 1.00 37.08 MOTA 3776 0 LEU 494 73.308 4.160 1.560 1.00 34.90 MOTA 3777 N ALA 495 73.839 2.779 3.243 1.00 37.18 MOTA 3779 CA ALA 495 75.246 2.830 2.918 1.00 39.84 MOTA 3780 CB ALA 495 75.885 4.066 3.541 1.00 39.29 MOTA 3781 С ALA 495 75.949 1.578 3.400 1.00 41.68 MOTA 3782 О ALA 495 75.400 0.808 4.189 1.00 41.53 MOTA 3783 N GLU 496 77.149 1.348 2.881 1.00 43.44 MOTA 3785 CA GLU 496 77.936 0.202 3.297 1.00 42.86 MOTA 3786 CB GLU 496 78.328 -0.663 2.101 1.00 44.63 3787 MOTA CG GLU 496 77.120 -1.167 1.320 1.00 53.31 3788 MOTA CD GLU 496 77.386 -2.450 0.545 1.00 59.48 ATOM 3789 OE1 GLU 496 76.494 -3.332 0.534 1.00 62.39 MOTA 3790 OE2 GLU 496 78.477 -2.580 -0.053 1.00 62.15 MOTA 3791 C GLU 496 79.150 0.750 4.006 1.00 40.96 MOTA 3792 0 GLU 496 79.889 1.568 3.455 1.00 40.81 MOTA 3793 N ALA 497 79.267 0.411 5.280 1.00 40.79 MOTA 3795 CA ALA 497 80.381 0.857 6.096 1.00 41.84 MOTA 3796 CB ALA 497 79.888 1.240 7.478 1.00 38.80 MOTA 3797 C ALA 497 81.394 -0.280 6.181 1.00 44.72 MOTA 3798 0 ALA 497 81.019 -1.445 6.215 1.00 44.78 MOTA 3799 N ILE 498 82.678 0.054 6.183 1.00 48.03 MOTA 3801 CA ILE 498 83.729 -0.952 6.255 1.00 48.78 MOTA 3802 CB ILE 498 84.654 -0.894 5.014 1.00 50.57 MOTA 3803 CG2 ILE 498 85.748 -1.954 5.119 1.00 51.32 MOTA 3804 CG1 ILE 498 83.851 -1.103 3.726 1.00 51.90 MOTA 3805 CD1 ILE 498 83.139 0.146 3.198 1.00 55.47 MOTA 3806 С ILE 498 84.573 -0.754 7.511 1.00 48.31 MOTA 3807 0 ILE 498 85.005 0.359 7.805 1.00 47.90 MOTA 3808 N GLY 499 84.754 -1.829 8.271 1.00 49.29 MOTA 3810 CA GLY 499 85.563 -1.774 9.479 1.00 53.17 ATOM 3811 С GLY 499 85.076 -0.944 10.657 1.00 57.22 ATOM 3812 0 GLY 499 85.885 -0.341 11.364 1.00 59.20 MOTA 3813 N LEU 500 83.768 -0.948 10.909 1.00 58.51 MOTA 3815 CA LEU 500 83.193 -0.189 12.025 1.00 57.80 ATOM 3816 CB LEU 500 81.705 -0.519 12.181 1.00 55.67

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MOTA 3817 CG LEU 500 80.789 0.036 11.086 1.00 54.81 ATOM 3818 CD1 LEU 500 79.361 -0.445 11.293 1.00 53.00 MOTA 3819 CD2 LEU 500 80.854 1.561 11.089 1.00 53.27 **ATOM** 3820 13.333 С LEU 500 83.926 -0.466 1.00 58.15 MOTA 3821 O LEU 500 -1.560 84.461 13.529 1.00 60.29 **ATOM** 3822 N **PRO** 505 87.397 -6.022 10.511 1.00 77.18 ATOM 3823 CD PRO 505 88.509 -6.651 11.242 1.00 78.26 ATOM 3824 CA **PRO** 505 87.755 -4.660 10.097 1.00 75.62 MOTA 3825 CB PRO 505 89.166 -4.487 10.669 1.00 75.77 **ATOM** 3826 CG PRO 505 89.696 -5.884 10.715 1.00 77.07 MOTA 3827 С PRO 505 87.709 -4.440 8.583 1.00 73.15 **ATOM** 3828 O PRO 505 87.772 -3.308 8.105 1.00 72.63 **ATOM** 3829 N **ASN** 506 87.595 -5.524 7.830 1.00 71.27 3831 MOTA CA ASN 506 87.518 -5.421 6.380 1.00 69.14 MOTA 3832 CB ASN 506 88.577 -6.313 5.728 1.00 70.76 **ATOM** 3833 C ASN 506 86.119 -5.840 5.940 1.00 67.30 **ATOM** 3834 O ASN 506 85.834 -5.957 4.750 1.00 67.03 MOTA 3835 N 507 ARG 85.250 -6.064 6.921 1.00 65.27 MOTA 3837 CA ARG 507 83.876 -6.479 6.669 1.00 62.B6 MOTA 3838 CB ARG 507 83.335 -7.267 7.864 1.00 65.45 MOTA 3839 C ARG 507 82.991 -5.274 6.443 1.00 59.56 ATOM 3840 0 ARG 507 83.161 -4.247 7.100 1.00 59.70 ATOM 3841 N VAL 508 82.057 -5.397 5.509 1.00 56.65 **ATOM** 3843 CA VAL 508 81.135 -4.310 5.226 1.00 55.48 MOTA 3844 CB VAL 508 80.850 -4.157 3.719 1.00 55.71 MOTA 3845 CG1 VAL 508 82.146 -3.962 2.962 1.00 58.18 MOTA 3846 CG₂ VAL 508 80.096 -5.356 3.188 1.00 58.76 MOTA 3847 C VAL 508 79.833 -4.537 5.979 1.00 53.10 **ATOM** 3848 0 VAL 508 79.352 -5.665 6.091 1.00 54.25 MOTA 3849 N THR 509 79.282 -3.460 6.514 1.00 50.06 MOTA 3851 CA THR 509 78.041 -3.512 7.260 1.00 45.70 MOTA 3852 CB THR 509 78.256 -3.029 8.715 1.00 45.59 MOTA 3853 OG1 THR 509 79.395 -3.696 9.279 1.00 43.86 THR **ATOM** 3855 CG2 509 77.028 -3.328 9.573 1.00 44.19 ATOM 3856 THR С 509 77.064 -2.574 6.564 1.00 43.57 MOTA 3857 509 0 THR 77.416 -1.444 6.221 1.00 41.15 MOTA 3858 N LYS 510 75.871 -3.073 6.268 1.00 42.96 **ATOM** 3860 CA LYS 510 -2.253 74.847 5.640 1.00 41.91 ATOM 3861 CB LYS 510 73.740 -3.144 5.091 1.00 44.74 MOTA 3862 CG LYS 510 72.864 -2.461 4.069 1.00 51.83 **ATOM** 3863 CDLYS 510 73.392 -2.645 2.659 1.00 55.00 MOTA 3864 CE LYS 510 72.769 -3.879 2.020 1.00 58.36 MOTA 3865 NZ LYS 510 73.069 -5.131 2.769 1.00 58.57 ATOM 3869 С LYS 510 74.322 -1.367 6.789 1.00 40.74 MOTA 3870 0 LYS 510 73.909 -1.874 7.837 1.00 40.26 MOTA 3871 -0.052 N VAL 511 74.413 1.00 6.624 37.21 MOTA 3873 CA VAL 511 73.989 0.877 7.661 1.00 33.44 MOTA 3874 CB VAL 511 75.227 1.515 8.362 1.00 34.53 **ATOM** 3875 CG1 VAL 511 76.100 0.436 9.014 1.00 31.98 **ATOM** 3876 CG2 VAL 511 76.048 2.322 7.358 1.00 34.82 MOTA 3877 C VAL 511 73.134 1.989 7.087 1.00 31.34 MOTA 3878 0 VAL 511 73.025 2.130 5.871 1.00 31.33 **ATOM** 3879 N ALA 512 72.485 2.748 7.961 1.00 30.70 ATOM 3881 CA ALA 512 71.671 3.876 7.523 1.00 30.81

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MOTA 3882 CB ALA 512 70.305 3.879 8.206 1.00 29.85 MOTA 3883 C ALA 512 72.453 5.124 7.904 1.00 31.30 MOTA 3884 ALA 0 512 73.036 5.197 8.996 1.00 30.24 **ATOM** 3885 N VAL 513 6.096 72.480 6.999 1.00 30.86 **ATOM** 3887 CA VAL 513 73.208 7.332 7.238 1.00 30.58 MOTA 3888 CB VAL 513 74.358 7.525 6.223 1.00 31.11 **ATOM** 3889 CG1 VAL 513 75.132 8.788 6.547 1.00 29.63 **ATOM** 3890 CG2 VAL 513 75.290 6.317 6.223 1.00 28.70 MOTA 3891 C VAL 513 72.300 8.556 7.189 1.00 31.28 **MOTA** 3892 0 VAL 513 71.645 8.824 6.167 1.00 30.12 **ATOM** 3893 N LYS 514 72.229 9.257 8.321 1.00 31.03 MOTA 3895 CA LYS 514 71.439 10.479 8.451 1.00 32.56 MOTA 3896 CB LYS 10.635 514 70.881 9.870 1.00 34.31 **ATOM** 3897 CG · LYS 514 69.977 9.516 10.326 1.00 38.25 MOTA 3898 CD LYS 514 69.513 9.774 11.753 1.00 47.74 MOTA 3899 CE LYS 514 68.514 8.719 12.230 1.00 51.60 MOTA 3900 NZ LYS 514 67.226 8.755 11.468 1.00 58.53 MOTA 3904 C LYS 514 72.357 11.659 8.137 1.00 30.29 ATOM 3905 0 LYS 514 73.485 11.736 8.628 1.00 28.14 ATOM 3906 N MET 515 71.867 12.580 7.320 1.00 30.67 MOTA 3908 CA MET 515 72.643 13.747 6.920 1.00 29.94 MOTA 3909 CB MET 515 73.435 13.442 5.648 1.00 30.64 MOTA 3910 CG MET 515 72.557 13.038 4.464 1.00 32.16 **ATOM** 3911 SD MET 515 73.525 12.522 3.036 1.00 37.59 **ATOM** 3912 CE MET 515 74.015 10.933 3.563 1.00 29.11 MOTA 3913 С MET 515 71.675 14.869 6.635 1.00 29.71 **ATOM** 3914 0 MET 515 70.462 30.04 14.664 6.598 1.00 MOTA 3915 N LEU 516 72.212 16.060 6.445 29.56 1.00 **MOTA** 3917 CA LEU 516 71.381 17.206 6.136 1.00 30.76 **ATOM** 3918 CB LEU 516 72.093 18.508 6.526 1.00 28.20 **ATOM** 3919 CG LEU 516 72.396 18.724 8.011 1.00 28.48 MOTA 3920 LEU CD1 516 73.202 19.983 8.185 1.00 27.55 **MOTA** 3921 CD2 LEU 516 71.114 18.814 8.794 1.00 25.49 **ATOM** 3922 C LEU 516 71.081 17.225 4.647 1.00 30.97 **ATOM** 3923 LEU 0 516 71.728 16.534 3.851 1.00 29.93 **ATOM** 3924 N LYS 517 70.030 17.946 4.291 1.00 31.57 **ATOM** 3926 CA LYS 517 69.677 18.117 2.899 1.00 31.44 MOTA 3927 CB LYS 517 68.169 2.752 18.310 1.00 34.79 **ATOM** 3928 CG LYS 517 67.375 17.098 3.194 1.00 38.42 **ATOM** 3929 CD LYS 517 66.148 16.888 2.343 1.00 46.52 **ATOM** 3930 CE LYS 517 65.087 17.950 2.582 1.00 53.77 MOTA 3931 NZ LYS 517 63.901 17.740 1.690 1.00 56.38 **ATOM** 3935 С LYS 517 70.457 19.377 2.499 1.00 30.18 ATOM 3936 0 LYS 517 70.892 20.134 3.370 1.00 27.47 **ATOM** 3937 N SER 518 70.646 19.594 1.201 1.00 31.13 **ATOM** 3939 CA 518 SER 71.394 20.747 0.693 1.00 32.11 **ATOM** 3940 CB SER 518 71.518 20.652 -0.824 1.00 33.45 **ATOM** 3941 0G SER 518 70.242 20.567 -1.428 1.00 34.51 MOTA 3943 C SER 518 70.814 22.103 1.073 1.00 32.81 **ATOM** 3944 0 SER 518 71.515 23.123 1.027 1.00 34.03 **ATOM** 3945 N ASP 519 69.540 22.117 1.449 1.00 29.80 MOTA 3947 CA **ASP** 519 68.886 23.354 1.836 1.00 28.94 ATOM 3948 CB **ASP** 519 67.473 23.421 1.237 1.00 33.90 MOTA 3949 CG **ASP** 519 66.542 22.332 1.771 1.00 34.42

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MOTA 3950 OD1 ASP 519 67.020 21.328 2.333 1.00 35.58 3951 MOTA OD2 ASP 519 65.313 22.485 1.617 1.00 41.83 **ATOM** 3952 C **ASP** 519 68.829 23.559 3.342 1.00 29.08 MOTA 3953 0 **ASP** 519 68.177 24.485 3.816 1.00 29.79 MOTA 3954 N ALA 520 69.514 22.710 4.099 1.00 29.73 MOTA 3956 CA ALA 520 69.488 22.824 1.00 5.558 29.16 3957 MOTA CB ALA 520 70.174 21.639 6.190 1.00 28.13 3958 MOTA C ALA 520 70.122 24.108 6.040 1.00 28.06 MOTA 3959 0 ALA 520 70.880 24.741 5.309 1.00 28.84 ATOM 3960 N THR 521 69.800 24.491 7.272 1.00 27.84 MOTA 3962 CA THR 521 70.357 25.692 7.885 1.00 30.45 MOTA 3963 CB THR 521 69.254 26.635 8.463 1.00 33.56 MOTA 3964 OG1 THR 521 68.547 25.968 9.520 1.00 36.27 MOTA 3966 CG2 THR 521 68.275 27.074 7.379 1.00 36.06 ATOM 3967 С THR 521 71.251 25.263 9.048 1.00 30.04 **ATOM** 3968 0 THR 521 71.348 24.072 9.369 1.00 28.16 MOTA 3969 N GLII 522 71.876 26.241 9.696 1.00 31.42 MOTA 3971 CA GLU 522 72.745 25.978 10.832 1.00 36.94 MOTA 3972 CB GLU 522 73.404 27.282 11.299 1.00 44.74 ATOM 3973 CG GLU 522 74.414 27.130 12.450 1.00 58.34 MOTA 3974 CD GLU 522 75.769 26.579 12.009 1.00 64.50 MOTA 3975 GLU 522 OE1 76.798 27.261 12.231 1.00 64.89 MOTA 3976 OE₂ GLU 522 75.806 25.461 11.452 1.00 70.26 MOTA 3977 С GLU 522 71.932 25.345 11.969 1.00 34.02 MOTA 3978 GLU 522 0 72.428 24.480 12.684 1.00 31.11 ATOM 3979 N LYS 523 70.670 25.750 12.097 1.00 32,53 ATOM 3981 CA LYS 523 69.805 25.210 13.135 1.00 34.06 MOTA 3982 CB LYS 523 68.481 25.970 13.188 1.00 39.54 MOTA 3983 CG LYS 523 67.560 25.541 14.322 1.00 45.55 MOTA 3984 CDLYS 523 66.360 24.776 13.789 1.00 52.08 **ATOM** 3985 LYS CE 523 65.443 24.312 14.914 1.00 54.16 ATOM 3986 NZ LYS 523 64.313 23.509 14.373 1.00 54.38 MOTA 3990 C LYS 523 69.572 23.733 12.861 1.00 31.73 MOTA 3991 0 LYS 523 69.589 22.922 13.788 1.00 31.15 MOTA 3992 ASP N 524 69.374 23.383 11.590 1.00 29.22 3994 **ATOM ASP** CA 524 69.182 21.980 11.214 1.00 28.79 MOTA 27.65 3995 CB ASP 524 68.928 21.831 9.714 1.00 MOTA 3996 CG ASP 524 67.586 22.396 9.286 1.00 33.89 MOTA 3997 OD1 ASP 524 66.568 22.106 9.954 34.66 1.00 ATOM 3998 OD2 **ASP** 524 67.549 23.120 8.270 1.00 30.04 **ATOM** 3999 С ASP 524 70.424 21.190 11.606 1.00 28.00 MOTA 4000 0 ASP 524 70.317 20.104 12.162 1.00 30.83 ATOM 4001 N LEU 525 71.603 21.761 11.347 1.00 29.87 **ATOM** 4003 CA LEU 525 72.873 21.121 11.700 1.00 27.60 MOTA 4004 CB LEU 525 74.064 21.997 11.282 1.00 24.08 MOTA 4005 CG LEU 525 75.462 21.433 11.593 1.00 26.11 MOTA 4006 CD1 LEU 525 75.597 19.979 11.098 1.00 23.67 MOTA 4007 CD2 LEU 525 76.530 22.321 10.967 1.00 21.28 ATOM 4008 C LEU 525 72.909 20.869 13.200 1.00 26.38 MOTA 4009 0 LEU 525 73.249 19.777 13.653 1.00 26.09 MOTA 4010 N SER 526 72.560 21.902 13.956 1.00 29.72 ATOM 4012 21.861 CA SER 526 72.500 15.422 1.00 32.16 MOTA 4013 CB SER 71.980 526 23.209 15.939 1.00 33.45 ATOM 4014 OG SER 526 71.793 23.213 17.343 1.00 40.42

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ATOM	4016	C	SER	526	71.572	20.728	15.902	1.00	31.64
ATOM	4017	0	SER	526	71.869	20.030	16.889	1.00	32.54
MOTA	4018	N	ASP	527	70.454	20.561	15.201	1.00	27.92
ATOM	4020	CA	ASP	527	69.492	19.527	15.524	1.00	28.60
ATOM	4021	CB	ASP	527	68.187	19.767	14.765	1.00	29.35
ATOM	4022	CG	ASP	527	67.418	20.984	15.278	1.00	31.37
ATOM	4023	OD1	ASP	527	67.759	21.549	16.353	1.00	31.96
ATOM	4024	OD2	ASP	527	66.456	21.369	14.591	1.00	32.58
MOTA	4025	С	ASP	527	70.038	18.131	15.246	1.00	28.82
ATOM	4026	0	ASP	527	69.854	17.212	16.047	1.00	29.65
MOTA	4027	N	LEU	528	70.721	17.962	14.120	1.00	29.29
ATOM	4029	CA	LEU	528	71.302	16.658	13.794	1.00	29.94
MOTA	4030	CB	LEU	528	71.780	16.621	12.336	1.00	26.45
ATOM	4031	CG	LEU	528	72.315	15.276	11.840	1:00	28.34
ATOM	4032	CD1	LEU	528	71.240	14.189	12.035	1.00	27.16
ATOM	4033	CD2	LEU	528	72.756	15.387	10.372	1.00	25.91
ATOM	4034	С	LEU	528	72.449	16.319	14.776	1.00	29.72
MOTA	4035	0	LEU	528	72.617	15.162	15.178	1.00	28.98
ATOM	4036	N	ILE	529	73.224	17.329	15.168	1.00	30.15
MOTA	4038	CA	ILE	529	74.305	17.131	16.134	1.00	28.88
ATOM	4039	CB	ILE	529	75.188	18.382	16.268	1.00	26.91
ATOM	4040	CG2	ILE	529	76.175	18.221	17.423	1.00	24.82
MOTA	4041	CG1	ILE	529	75.960	18.613	14.984	1.00	23.98
ATOM	4042	CD1	ILE	529	76.663	19.932	14.973	1.00	28.33
ATOM	4043	С	ILE	529	73.709	16.799	17.518	1.00	29.71
ATOM	4044	0	ILE	529	74.172	15.880	18.193	1.00	29.19
ATOM	4045	N	SER	530	72.672	17.524	17.926	1.00	26.84
ATOM	4047	CA	SER	530	72.061	17.247	19.214	1.00	31.46
ATOM	4048	CB	SER	530	70.948	18.251	19.521	1.00	36.17
MOTA	4049	OG	SER	530	70.045	18.363	18.431	1.00	47.58
MOTA	4051	C	SER	530	71.526	15.822	19.248	1.00	30.05
ATOM	4052	0	SER	530	71.646	15.136	20.270	1.00	29.61
MOTA	4053	N	GLU	531	70.972	15.357	18.132	1.00	27.74
MOTA	4055	CA	GLU	531	70.458	13.999	18.090	1.00	28.71
MOTA	4056	CB	GLU	531	69.709	13.727	16.789	1.00	29.72
MOTA	4057	CG	GLU	531	69.147	12.319	16.737	1.00	32.21
MOTA	4058	CD	GLU	531	68.510	11.979	15.414	1.00	33.88
MOTA	4059	OE1	GLU	531	68.026	10.846	15.281	1.00	37.60
ATOM	4060	OE2	GLU	531	68.483	12.833	14.510	1.00	34.70
ATOM	4061	C	GLU	531	71.578	12.974	18.271	1.00	28.91
ATOM	4062	0	GLU	531	71.428	12.007	19.019	1.00	29.46
ATOM	4063	N	MET	532	72.686	13.179	17.567	1.00	28.84
ATOM	4065	CA	MET	532	73.851	12.296	17.648	1.00	29.35
ATOM	4066	CB	MET	532	74.948	12.786	16.689	1.00	27.41
MOTA	4067	CG	MET	532	76.299	12.117	16.872	1.00	26.71
MOTA	4068	SD	MET	532	77.503	12.675	15.640	1.00	32.27
MOTA	4069	CE	MET	532	77.732	14.400	16.117	1.00	24.10
MOTA	4070	С	MET	532	74.389	12.280	19.078	1.00	28.80
ATOM	4071	0	MET	532	74.700	11.230	19.630	1.00	29.74
MOTA	4072	N	GLU	533	74.481	13.454	19.681	1.00	28.83
ATOM	4074	CA	GLU	533	74.985	13.546	21.033	1.00	29.66
MOTA	4075	СВ	GLU	533	75.182	15.008	21.423	1.00	32.23
MOTA	4076	CG	GLU	533	76.331	15.687	20.651	1.00	34.47
MOTA	4077	CD	GLU	533	77.656	14.937	20.774	1.00	38.03
									20.03

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MOTA 4078 OE1 GLU 533 78.168 14.780 21.903 1.00 39.75 MOTA 4079 OE2 GLU 533 78.192 14.497 19.736 1.00 38.75 MOTA 4080 C GLU 533 74.058 12.815 22.005 1.00 31.55 MOTA 4081 0 GLU 533 74.521 12.083 22.889 1.00 30.63 **ATOM** 4082 MET 534 72.750 12.958 21.799 1.00 N 31.31 **ATOM** 4084 CA MET 534 71.789 12.289 22.664 1.00 30.78 12.672 MOTA 4085 CB MET 70.348 1.00 534 22.319 31.23 **ATOM** 4086 CG MET 69.453 534 12.648 23.551 0.50 29.35 PRT1 **ATOM** 4087 SD 67.688 MET 534 12.563 23.246 0.50 28.79 PRT1 **ATOM** 4088 CE MET 534 67.290 14.230 22.875 0.50 26.96 PRT1 MOTA 4089 C MET 534 71.991 10.773 22.560 1.00 28.82 ATOM 4090 0 MET 534 72.053 10.083 23.568 1.00 30.10 MOTA 4091 N MET 535 72.149 10.271 21.339 1.00 29.16 MOTA CA 72.381 4093 MET 535 8.852 21.110 1.00 29.37 **ATOM** 4094 535 72.546 CB MET 8.551 19.617 1.00 27.35 MOTA 4095 CG MET 535 71.281 8.790 18.817 1.00 28.40 **ATOM** 4096 SD MET 535 71.255 7.955 17.255 1.00 30.26 **ATOM** 4097 CE MET 535 71.336 9.279 16.188 1.00 35.50 MOTA 4098 С MET 535 73.612 1.00 8.388 21.887 30.36 MOTA 4099 O MET 535 73.626 7.287 22.460 1.00 26.13 MOTA 4100 N LYS 536 74.640 9.233 21.909 1.00 30.70 MOTA 4102 CA LYS 536 75.850 8.913 22.649 1.00 31.76 MOTA 4103 CB LY\$ 536 76.934 9.954 22.388 1.00 31.05 MOTA 4104 CG LYS 536 77.550 9.883 21.004 1.00 26.80 **ATOM** 4105 CDLYS 536 78.534 11.017 20.860 1.00 31.05 MOTA 4106 CE LYS 536 79.132 11.138 19.466 1.00 29.83 MOTA 4107 NZ LYS 536 79.957 12.377 19.440 1.00 29.32 MOTA 4111 C LYS 536 75.550 8.834 24.150 1.00 31.99 **ATOM** 4112 0 LYS 536 75.920 7.859 24.806 1.00 31.92 MOTA 4113 N MET 537 74.837 9.826 24.676 1.00 31.81 MOTA 4115 CA MET 537 74.517 9.835 26.090 1.00 35.37 ATOM 4116 CB 537 MET 73.860 11.154 26.506 1.00 41.32 **ATOM** 4117 CG MET 537 74.828 12.335 26.610 1.00 51.50 **ATOM** 4118 SD MET 537 76.234 12.090 27.776 1.00 57.48 MOTA 4119 CE MET 537 75.460 12.637 29.334 1.00 56.91 **ATOM** 4120 C MET 537 73.630 8.679 26.499 1.00 36.11 **ATOM** 8.084 4121 0 MET 537 73.845 27.548 1.00 38.54 MOTA 4122 N ILE 538 72.652 8.347 25.661 1.00 33.69 **ATOM** CA ILE 4124 538 71.704 7.277 25.954 1.00 31.62 MOTA 4125 CB ILE 538 70.492 7.314 24.974 1.00 28.21 MOTA 4126 CG2 ILE 538 69.681 6.013 25.034 1.00 28.22 ATOM 4127 CG1 ILE **538** 69.590 8.488 25.338 1.00 23.74 ATOM 4128 CD1 ILE 538 68.487 8.728 24.344 1.00 27.94 MOTA 4129 C 1.00 ILE 538 72.322 5.894 26.008 31.07 MOTA 4130 0 ILE 538 71.952 26.860 5.080 1.00 33.13 MOTA 4131 N GLY 539 73.239 5.611 25.094 1.00 29.52 MOTA 4133 CA GLY 539 73.871 4.309 25.093 1.00 28.40 MOTA 4134 C GLY 539 73.111 3.275 24.289 1.00 30.21 MOTA 4135 0 GLY 539 72.018 3.554 23.788 1.00 29.66 MOTA 4136 N LYS 540 73.679 2.074 24.199 1.00 28.44 MOTA 4138 CA LYS 540 73.105 0.984 1.00 31.09 23.426 MOTA 4139 CB LYS 540 74.215 0.089 22.895 1.00 33.15 MOTA CG 540 4140 LYS 75.116 0.776 21.906 1.00 39.54 ATOM 4141 CD LYS 540 76.125 -0.175 21.329 1.00 43.98

ATOM	4142	CE.	LYS	540	77.033	0.562	20.349	1.00	50.79
MOTA	4143	NZ	LYS	540	76.338	0.977	19.086	1.00	51.09
MOTA	4147	С	LYS	540	72.053	0.087	24.059	1.00	32.78
ATOM	4148	0	LYS	540	72.088	-0.195	25.266	1.00	32.41
MOTA	4149	N	HIS	541	71.137	-0.374	23.208	1.00	31.20
MOTA	4151	CA	HIS	541	70.080	-1.304	23.591	1.00	31.53
MOTA	4152	CB	HIS	541	68.911	-0.630	24.298	1.00	30.69
MOTA	4153	CG	HIS	541	67.948	-1.613	24.882	1.00	31.18
MOTA	4154	CD2	HIS	541	67.938	-2.255	26.072	1.00	33.02
MOTA	4155	ND1	HIS	541	66.882	-2.123	24.165	1.00	30.56
MOTA	4157	CE1	HIS	541	66.268	-3.037	24.889	1.00	32.95
MOTA	4158	NE2	HIS	541	66.886	-3.140	26.053	1.00	31.79
MOTA	4160	C	HIS	541	69.590	-2.013	22.340	1.00	32.72
MOTA	4161	0	HIS	541	69.495	-1.404	21.275	1.00	30.34
MOTA	4162	N	LYS	542	69.282	-3.305	22.475	1.00	32.32
MOTA	4164	CA	LYS	542	68.828	-4.131	21.359	1.00	30.29
MOTA	4165	CB	LYS	542	68.637	-5.587	21.798	1.00	29.34
MOTA	4166	C	LYS	542	67.560	-3.661	20.692	1.00	29.09
MOTA	4167	0	LYS	542	67.369	-3.903	19.507	1.00	29.12
MOTA	4168	N	ASN	543	66.683	-3.012	21.446	1.00	28.54
MOTA	4170	CA	ASN	543	65.425	-2.559	20.869	1.00	29.10
MOTA	4171	CB	ASN	543	64.245	-3.047	21.712	1.00	29.69
ATOM	4172	CG	ASN	543	64.253	-4.556	21.900	1.00	29.62
ATOM	4173	OD1	ASN	543	64.510	-5.050	23.000	1.00	31.63
MOTA	4174	ND2	ASN	543	64.020	-5.291	20.828	1.00	28.66
MOTA	4177	С	ASN	543	65.299	-1.073	20.532	1.00	29.61
MOTA	4178	0	ASN	543	64.207	-0.507	20.578	1.00	28.00
MOTA	4179	N	ILE	544	66.432	-0.442	20.222	1.00	28.39
MOTA	4181	CA	ILE	544	66.466	0.958	19.804	1.00	25.73
MOTA	4182	CB	ILE	544	66.903	1.952	20.935	1.00	25.98
MOTA	4183	CG2	ILE	544	66.083	1.721	22.215	1.00	22.04
ATOM	4184	CG1	ILE	544	68.412	1.860	21.209	1.00	24.30
MOTA	4185	CD1	ILE	544	68.901	2.846	22.274	1.00	22.83
ATOM	4186	C	ILE	544	67.463	1.020	18.639	1.00	26.20
MOTA	4187	0	ILE	544	68.276	0.106	18.467	1.00	25.46
ATOM	4188	N	ILE	545	67.307	2.016	17.771	1.00	26.26
MOTA	4190	CA	ILE	545	68.223	2.209	16.641	1.00	27.62
MOTA	4191	CB	ILE	545	67.647	3.195	15.585	1.00	28.33
ATOM	4192	CG2	ILE	545	68.726	3.595	14.562	1.00	28.00
MOTA	4193	CG1	ILE	545	66.453	2.565	14.856	1.00	24.69
ATOM	4194	CD1	ILE	545	66.850	1.467	13.875	1.00	26.17
MOTA	4195	С	ILE	545	69.492	2.794	17.267	1.00	28.23
MOTA	4196	0	ILE	545	69.468	3.872	17.846	1.00	28.97
MOTA	4197	N	ASN	546	70.595	2.069	17.164	1.00	29.45
MOTA	4199	CA	ASN	546	71.845	2.508	17.774	1.00	28.58
MOTA	4200	CB	ASN	546	72.580	1.309	18.384	1.00	26.34
MOTA	4201	CG	ASN	546	71.812	0.673	19.527	1.00	25.52
MOTA	4202	OD1	ASN	546	71.634	1.277	20.580	1.00	28.82
MOTA	4203	ND2	ASN	546	71.341	-0.542	19.318	1.00	26.57
ATOM	4206	C	ASN	546	72.810	3.264	16.881	1.00	28.74
ATOM	4207	0	ASN	546	72.858	3.041	15.675	1.00	29.26
MOTA	4208	N	LEU	547	73.578	4.155	17.504	1.00	29.90
ATOM	4210	CA	LEU	547	74.618	4.936	16.834	1.00	30.27
ATOM	4211	CB	LEU	547	75.075	6.081	17.745	1.00	25.85

1.00 MOTA 4212 CG LEU 547 76.161 7.034 17.232 27.73 MOTA 4213 CD1 LEU 547 75.670 7.851 16.033 1.00 27.38 MOTA 4214 CD2 LEU 547 76.545 7.966 18.345 1.00 29.14 MOTA 4215 С LEU 547 75.811 4.004 16.567 1.00 32.22 MOTA 4216 0 LEU 547 76.256 3.291 17.471 1.00 33.38 ATOM 4217 LEU N 548 76.317 4.005 15.335 1.00 32.12 ATOM 4219 CA LEU 548 77.452 3.159 14.960 1.00 32.94 MOTA 4220 CB LEU 548 77.103 2.310 13.740 1.00 29.97 MOTA 4221 CG LEU 548 75.839 1.458 13.840 1.00 31.55 **MOTA** 4222 CD1 LEU 548 75.662 0.713 12.540 1.00 27.85 MOTA 4223 CD2 LEU 54B 75.917 0.500 15.025 1.00 26.34 **ATOM** 4224 C LEU 548 78.726 3.955 14.654 1.00 36.06 4225 ATOM 0 LEU 548 79.836 3.410 14.668 1.00 36.42 4226 MOTA N GLY 549 78.562 5.219 14.298 ... 1.00 35.78 MOTA 4228 CA GLY 549 79.713 6.042 13.987 1.00 36.22 **ATOM** 4229 C GLY 549 79.267 7.376 13.433 1.00 35.30 ATOM 4230 0 GLY 549 78.062 7.646 13.362 1.00 33.46 MOTA 4231 N ALA 550 80.232 8.206 13.042 1.00 34.94 MOTA 4233 CA ALA 550 12.490 79.945 9.525 1.00 31.91 MOTA 4234 CB ALA 550 79.588 10.495 13.613 1.00 30.54 ATOM 4235 C ALA 550 81.128 10.077 11.715 1.00 31.58 **ATOM** 4236 ALA 0 550 82.281 9.832 12.080 1.00 31.23 **ATOM** 4237 N CYS 551 80.818 10.812 10.643 1.00 31.13 **ATOM** 4239 CA CYS 551 81.805 11.503 9.804 1.00 28.28 **ATOM** 4240 CB CYS 551 81.621 11.180 8.316 1.00 27.27 MOTA 4241 SG CYS 551 81.771 7.839 1.00 9.449 30.33 MOTA 4242 C CYS 551 81.450 12.960 10.074 1.00 25.88 MOTA 4243 0 CYS 551 80.432 13.458 9.605 1.00 27.73 MOTA 4244 N THR 552 82.214 13.586 10.954 1.00 25.35 MOTA 4246 CA THR 552 81.988 14.967 11.353 1.00 26.79 MOTA 4247 CB THR 552 82.051 15.092 12.899 1.00 27.76 MOTA 4248 OG1 THR 552 83.392 14.839 13.338 1.00 27.62 MOTA 4250 CG₂ THR 552 81.119 14.086 13.575 1.00 29.17 MOTA 4251 C THR 552 83.036 15.931 10.790 1.00 25.03 MOTA 4252 0 THR 552 82.825 10.746 17.137 1.00 25.34 MOTA 4253 N GLN 84.174 553 15.385 10.381 1.00 27.34 MOTA 4255 CA GLN 553 85.285 16.190 9.888 1.00 26.31 MOTA 4256 CB GLN 553 86.601 15.639 10.468 1.00 25.05 ATOM 4257 CG GLN 553 86.581 15.491 11.993 1.00 24.78 MOTA 4258 CD GLN 553 86.382 16.823 12.709 1.00 25.40 MOTA 4259 OE1 GLN 553 87.175 17.748 12.546 1.00 33.74 MOTA 4260 NE2 GLN 85.338 553 16.920 13.516 1.00 25.61 MOTA 4263 C GLN 553 85.390 16.274 8.379 1.00 27.08 MOTA 4264 0 GLN 85.083 553 15.318 7.669 1.00 28.76 **ATOM** 4265 N ASP 85.804 554 17.438 7.899 1.00 28.63 **ATOM** 4267 CA ASP 86.015 554 17.677 6.471 1.00 29.70 MOTA 4268 CB ASP 554 87.335 17.050 6.051 1.00 29.73 MOTA 4269 CG ASP 554 88.480 17.587 6.857 1.00 33.38 MOTA 4270 OD1 ASP 554 88.794 18.780 6.711 1.00 36.53 ATOM 4271 OD2 ASP 554 89.024 16.841 7.687 1.00 36.40 **ATOM** 4272 С ASP 554 84.908 17.258 5.522 1.00 29.64 MOTA 4273 ASP 0 554 85.112 16.422 4.643 1.00 32.06 ATOM 4274 N GLY 555 83.748 17.881 5.679 1.00 28.59 MOTA 4276 CA GLY 555 82.620 17.579 4.825 1.00 26.85

ATOM	4277	С	GLY	555	81.333	17.434	5.607	1.00	25.30
MOTA	4278	0	GLY	555	81.319	17.593	6.834	1.00	23.96
ATOM	4279	N	PRO	556	80.229	17.113	4.920	1.00	24.84
MOTA	4280	CD	PRO	556	80.159	16.850	3.472	1.00	21.36
ATOM	4281	CA	PRO	556	78.920	16.942	5.550	1.00	25.26
ATOM	4282	CB	PRO	556	78.033	16.494	4.386	1.00	23.37
MOTA	4283	CG	PRO	556	79.025	15.881	3.398	1.00	24.44
ATOM	4284	С	PRO	556	78.885	15.941	6.700	1.00	26.50
MOTA	4285	0	PRO	556	79.515	14.875	6.654	1.00	27.38
MOTA	4286	N	LEU	557	78.171	16.314	7.754	1.00	26.25
ATOM	4288	CA	LEU	557	78.032	15.452	8.917	1.00	28.25
ATOM	4289	CB	LEU	557	77.403	16.217	10.092	1.00	27.09
ATOM	4290	CG	LEU	557	76.922	15.414	11.310	1.00	28.35
ATOM	4291	CD1	LEU	-557:-	78¥088	14.733	12.011	1.00	25.54
ATOM	4292	CD2	LEU	557	76.204	16.340	12.271	1.00	26.91
ATOM	4293	С	LEU	557	77.169	14.246	8.554	1.00	29.06
ATOM	4294	0	LEU	557	76.060	14.385	8.011	1.00	29.05
ATOM	4295	N	TYR	558	77.717	13.065	8.807	1.00	29.43
MOTA	4297	CA	TYR	558	77.018	11.823	8.573	1.00	28.02
ATOM	4298	CB	TYR	558	77.813	10.918	7.632	1.00	27.83
MOTA	4299	CG	TYR	558	77.969	11.414	6.203	1.00	31.70
MOTA	4300	CD1	TYR	558	78.966	10.893	5.383	1.00	32.90
ATOM	4301	CE1	TYR	558	79.121	11.315	4.073	1.00	32.69
MOTA	4302	CD2	TYR	558	77.122	12.386	5.666	1.00	30.23
MOTA	4303	CE2	TYR	558	77.271	12.815	4.350	1.00	29.97
ATOM	4304	CZ	TYR	558	78.280	12.272	3.560	1.00	33.20
ATOM	4305	OH	TYR	558	78.452	12.681	2.253	1.00	35.32
MOTA	4307	С	TYR	558	76.848	11.131	9.932	1.00	28.42
ATOM	4308	0	TYR	558	77.823	10.902	10.647	1.00	27.81
ATOM	4309	N	VAL	559	75.601	10.870	10.313	1.00	29.20
ATOM	4311	CA	VAL	559	75.286	10.175	11.564	1.00	29.17
ATOM	4312	CB	VAL	559	74.102	10.832	12.329	1.00	28.53
MOTA	4313	CG1	VAL	559	73.802	10.036	13.607	1.00	27.08
ATOM	4314	CG2	VAL	559	74.456	12.281	12.687	1.00	23.27
ATOM	4315	С	VAL	559	74.911	8.772	11.137	1.00	26.41
MOTA	4316	0	VAL	559	73.834	8.536	10.593	1.00	25.91
ATOM	4317	N	ILE	560	75.824	7.846	11.371	1.00	26.71
ATOM	4319	CA	ILE	560	75.638	6.465	10.966	1.00	27.55
MOTA	4320	CB	ILE	560	77.012	5.829	10.619	1.00	28.48
ATOM	4321	CG2	ILE	560	76.819	4.468	9.979	1.00	29.18
ATOM	4322	CG1	ILE	560	77.793	6.745	9.657	1.00	27.99
ATOM	4323	CD1	ILE	560	79.274	6.399	9.525	1.00	28.97
MOTA	4324	C	ILE	560	74.917	5.644	12.034	1.00	29.17
MOTA	4325	0	ILE	560	75.404	5.497	13.160	1.00	28.92
ATOM	4326	N	VAL	561	73.743	5.129	11.681	1.00	28.60
ATOM	4328	CA	VAL	561	72.957	4.325	12.606	1.00	28.58
ATOM	4329	CB	VAL	561	71.634	5.061	13.047	1.00	27.53
ATOM	4330	CG1	VAL	561	71.951	6.400	13.701	1.00	22.44
ATOM	4331	CG2	VAL	561	70.697	5.246	11.874	1.00	23.19
ATOM	4332	C	VAL	561	72.618	2.956	12.006	1.00	28.20
MOTA	4333	0	VAL	561	72.875	2.694	10.825	1.00	27.99
ATOM	4334	N	GLU	562	72.057	2.079	12.834	1.00	29.17
ATOM	4336	CA	GLU	562	71.666	0.744	12.399	1.00	28.96
MOTA	4337	CB	GLU	562	71.199	-0.086	13.589	1.00	27.34

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ATOM 4338 CG GLU 562 72.308 -0.331 14.583 1.00 30.12 MOTA 4339 1.00 CD GLU 562 71.838 -1.075 15.808 32.29 MOTA 4340 OE1 **GLU** 562 72.526 -2.030 16.217 1.00 32.45 -0.702 MOTA 4341 OE2 GLU 562 70.785 1.00 30.16 16.362 MOTA 4342 С GLU 562 70.580 0.794 1.00 11.340 29.79 MOTA 4343 GLU 0 562 69.690 1.653 11.386 1.00 29.75 MOTA 4344 N TYR 563 -0.106 1.00 70.684 10.369 30.51 MOTA 4346 CA TYR 563 69.735 -0.209 9.267 1.00 33.76 **ATOM** 4347 CB TYR 563 70.494 -0.602 7.988 1.00 31.04 **ATOM** 4348 CG TYR 563 69.624 -0.928 6.806 1.00 33.40 **ATOM** 4349 CD1 TYR 563 68.693 -0.019 6.340 1.00 33.07 MOTA 4350 CE1 TYR 563 67.908 -0.301 5.240 1.00 34.71 **ATOM** 4351 CD2 TYR 563-69.749 -2.141 6.147 1.00 34.61 **ATOM** 4352 CE2 TYR 563 68.970 -2.446 5.035 1.00 36.54 MOTA 4353 CZ TYR 563 68.047 -1.518 4.589 1.00 36.83 MOTA 4354 OH TYR 563 67.261 -1.805 3.501 1.00 38.81 ATOM 4356 C TYR 563 68.655 -1.269 9.588 1.00 36.14 MOTA 4357 0 TYR 563 68.946 -2.365 10.023 1.00 37.70 MOTA 4358 N ALA 564 67.406 -0.948 9.309 1.00 37.87 MOTA 4360 CA ALA 564 66.276 ~1.832 9.534 1.00 38.49 MOTA 4361 CB ALA 564 65.278 -1.167 10.458 1.00 42.57 ATOM 4362 С ALA 564 65.645 -2.153 8.179 1.00 39.65 MOTA 4363 ALA 0 564 64.796 -1.423 7.687 1.00 39.74 SER MOTA 4364 N 565 66.039 -3.280 7.607 1.00 40.06 MOTA CA 4366 SER 565 65.567 -3.699 6.295 1.00 40.67 MOTA 4367 CB SER 565 66.267 -4.986 5.883 1.00 38.71 MOTA 4368 OG SER 565 66.107 -5.964 6.889 1.00 41.35 ATOM 4370 С SER 565 64.081 -3.884 6.106 1.00 42.17 MOTA 4371 0 SER 565 63.585 4.992 -3.741 1.00 44.25 MOTA 4372 LYS N 566 63.360 -4.207 7.167 1.00 41.71 MOTA 4374 CA LYS 566 61.928 -4.427 7.015 1.00 40.22 MOTA 4375 CB LYS 7.800 566 61.525 -5.668 1.00 39.51 MOTA 4376 CG LYS 566 62.202 -6.910 7.226 1.00 41.48 MOTA 4377 CDLYS 566 62.113 -B.094 8.149 1.00 41.53 MOTA 4378 CE LYS 566 62.710 -9.312 7.491 1.00 41.18 MOTA 4379 NZ LYS 566 62.763 -10.458 8.438 1.00 46.17 MOTA 4383 С LYS 566 61.007 7.263 -3.220 1.00 40.47 MOTA 4384 0 LYS 59.800 566 -3.367 7.486 1.00 42.68 MOTA 4385 N GLY 1.00 38.90 567 61.584 -2.026 7.167 MOTA 4387 CA GLY 567 60.826 -0.799 7.336 1.00 37.13 MOTA 4388 GLY C 567 60.199 8.694 -0.592 1.00 36.72 MOTA 4389 O GLY 567 60.644 9.683 ~1.172 1.00 38.48 MOTA 4390 N ASN 568 59.191 0.273 8.753 1.00 35.77 MOTA 4392 CA ASN 568 58.518 10.015 0.549 1.00 35.36 MOTA 4393 CB ASN 568 57.883 1.957 10.045 1.00 36.30 MOTA 4394 CG ASN 568 56.635 2.088 9.169 1.00 38.06 MOTA 4395 OD1 ASN 568 55.623 9.383 1.00 1.421 38.66 MOTA 4396 ND2 ASN 568 56.686 3.010 8.221 1.00 37.29 MOTA 4399 С ASN 568 57.504 -0.532 10.341 1.00 33.04 MOTA 4400 ASN 0 568 57.061 -1.265 9.461 1.00 32.10 **ATOM** 4401 N LEU 569 57.142 -0.612 11.617 1.00 33.59 MOTA 4403 CA LEU 569 56.199 -1.604 12.132 1.00 32.91 MOTA 4404 CB LEU 569 56.045 -1.428 13.647 1.00 33.84 MOTA 4405 CG LEU 569 55.088 -2.343 14.403 1.00 31.96

SSSD/55145. v01

ATOM	4406	CD1	LEU	569	55.522	-3.797	14.216	1.00	33.20
ATOM	4407	CD2	LEU	569	55.089	-1.967	15.868	1.00	30.81
MOTA	4408	С	LEU	569	54.820	-1.591	11.478	1.00	32.12
MOTA	4409	0	LEU	569	54.214	-2.645	11.300	1.00	33.08
MOTA	4410	N	ARG	570	54.315	-0.409	11.148	1.00	32.05
MOTA	4412	CA	ARG	570	52.999	-0.293	10.529	1.00	35.21
MOTA	4413	CB	ARG	570	52.659	1.173	10.256	1.00	36.77
MOTA	4414	CG	ARG	570	51.282	1.370	9.653	1.00	43.11
ATOM	4415	CD	ARG	570	51.203	2.690	8.926	1.00	49.24
ATOM	4416	NE	ARG	570	52.154	2.775	7.815	1.00	55.77
ATOM	4418	CZ	ARG	570	52.995	3.790	7.619	1.00	58.89
ATOM	4419	NH1	ARG	570	53.016	4.820	8.463	1.00	61.61
ATOM	4422	NH2	ARG	570	53.804	3.786	6.566	1.00	59.16
ATOM	4425	С	ARG	570	52.992	-1.063	9.220	1.00	35.16
MOTA	4426	0	ARG	570	52.145	-1.922	8.990	1.00	35.50
ATOM	4427	N	GLU	571	53.971	-0.760	8.383	1.00	36.29
ATOM	4429	CA	GLU	571	54.111	-1.400	7.089	1.00	37.51
ATOM	4430	СВ	GLU	571	55.219	-0.701	6.308	1.00	41.27
ATOM	4431	CG	GLU	571	54.945	0.778	6.110	1.00	49.88
ATOM	4432	CD	GLU	571	56.087	1.516	5.436	1.00	57.58
ATOM	4433	OE1	GLU	571	57.264	1.122	5.636	1.00	60.59
ATOM	4434	OE2	GLU	571	55.804	2.504	4.714	1.00	61.14
ATOM	4435	С	GLU	571	54.399	-2.896	7.228	1.00	36.24
ATOM	4436	O	GLU	571	53.889	-3.716	6.459	1.00	34.22
ATOM	4437	N	TYR	572	55.202	-3.238	8.232	1.00	35.98
ATOM	4439	CA	TYR	572	55.570	-4.619	8.517	1.00	35.34
ATOM	4440	CB	TYR	572	56.526	-4.656	9.714	1.00	30.94
ATOM	4441	CG	TYR	572	56.959	-6.034	10.180	1.00	32.71
ATOM	4442	CD1	TYR	572	58.009	-6.714	9.547	1.00	32.33
MOTA	4443	CE1	TYR	572	58.464	-7.940	10.026	1.00	30.31
MOTA	4444	CD2	TYR	572	56.369	-6.626	11.303	1.00	33.43
MOTA	4445	CE2	TYR	572	56.813	-7.851	11.791	1.00	31.46
MOTA	4446	CZ	TYR	572	57.864	-8.502	11.148	1.00	33.99
ATOM	4447	ОН	TYR	572	58.311	-9.706	11.640	1.00	36.30
ATOM	4449	С	TYR	572	54.312	-5.425	8.826	1.00	37.26
ATOM	4450	0	TYR	572	54.121	-6.530	8.314	1.00	36.91
ATOM	4451	N	LEU	573	53.457	-4.850	9.665	1.00	36.82
ATOM	4453	CA	LEU	573	52.208	-5.476	10.075	1.00	35.56
MOTA	4454	CB	LEU	573	51.537	-4.629	11.165	1.00	34.03
MOTA	4455	CG	LEU	573	52.238	-4.527	12.519	1.00	32.82
MOTA	4456	CD1	LEU	573	51.621	-3.423	13.377	1.00	28.95
ATOM	4457	CD2	LEU	573	52.168	-5.858	13.207	1.00	29.46
ATOM	4458	С	LEU	573	51.237	-5.658	8.915	1.00	34.56
ATOM	4459	0	LEU	573	50.670	-6.729	8.726	1.00	34.80
ATOM	4460	N	GLN	574	51.030	-4.602	8.150	1.00	37.10
ATOM	4462	CA	GLN	574	50.101	-4.666	7.031	1.00	41.15
ATOM	4463	CB	GLN	574	49.875	-3.278	6.457	1.00	41.63
MOTA	4464	CG	GLN	574	49.089	-2.375	7.366	1.00	43.13
ATOM	4465	CD	GLN	574	49.063	-0.959	6.860	1.00	47.77
MOTA	4466	OE1	GLN	574	49.655	-0.647	5.827	1.00	50.00
ATOM	4467	NE2	GLN	574	48.378	-0.086	7.582	1.00	49.67
ATOM	4470	С	GLN	574	50.529	-5.627	5.934	1.00	42.38
ATOM	4471	0	GLN	574	49.685	-6.284	5.318	1.00	44.56
ATOM	4472	N	ALA	575	51.835	-5.717	5.697	1.00	41.99

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4474 575 52.367 4.676 1.00 41.29 ATOM CA ALA -6.608 MOTA 4475 CB ALA 575 53.841 -6.325 4.446 1.00 40.43 MOTA 4476 С 41.42 ALA 575 52.186 -8.058 5.066 1.00 4477 MOTA 0 ALA 575 4.249 1.00 43.65 52.392 -8.949 MOTA 4478 N ARG 576 51.815 -8.294 6.319 1.00 42.56 MOTA 4480 CA ARG 576 51.642 -9.646 6.824 1.00 42.51 MOTA 4481 CB ARG 52.676 7.920 1.00 576 -9.910 40.14 MOTA 4482 CG ARG 576 54.100 -9.896 7.377 1.00 40.32 MOTA 4483 CD ARG 576 55.172 -9.836 8.460 1.00 40.78 NE ATOM 4484 ARG 576 56.513 -9.783 7.874 1.00 42.13 4486 MOTA CZARG 576 56.975 -8.785 7.120 1.00 40.73 MOTA 4487 NH1 ARG 576 -7.732 56.215 6.851 1.00 39.21 MOTA 4490 NH2 ARG 576 58.201 -B.846 1.00 6.622 37.62 . MOTA 4493 С ARG 576 50.242 _ -9.931 1.00 7.326 44.48 MOTA 4494 0 ARG 576 -10.869 1.00 50.028 8.098 46.84 MOTA 4495 N ARG 577 49.275 -9.146 6.866 1.00 46.26 4497 ATOM CA ARG 577 47.893 -9.344 7.292 1.00 46.89 6.845 MOTA 4498 CB ARG 577 47.027 -8.170 1.00 46.16 ATOM 4499 CG 577 1.00 ARG 47.189 -6.939 7.696 44.93 MOTA 4500 CD ARG 577 46.463 -5.766 7.080 1.00 44.60 MOTA 4501 NE ARG 577 46.284 -4.683 8.039 1.00 45.05 MOTA 4503 CZ ARG 577 45.612 -3.565 7.793 1.00 45.95 MOTA 4504 NH1 ARG 577 45.052 -3.372 6.606 1.00 47.39 **ATOM** 4507 NH2 ARG 577 -2.655 1.00 45.466 8.749 45.49 MOTA 4510 C ARG 577 47.334 -10.649 6.740 1.00 46.60 MOTA 4511 0 ARG 577 47.478 -10.933 5.551 1.00 47.15 MOTA 4512 N GLN 594 53.312 -14.007 7.967 1.00 63.97 MOTA 4514 CA GLN 594 52.110 -14.068 8.799 1.00 63.06 MOTA 4515 CB GLN 594 51.175 -15.183 8.319 1.00 64.16 MOTA 4516 С GLN 594 52.501 -14.278 10.258 1.00 61.68 MOTA 4517 0 GLN 594 53.101 -15.292 10.619 1.00 60.95 ATOM 4518 N LEU 52.140 -13.313 11.092 1.00 595 58.58 MOTA 4520 CA LEU 52.470 -13.335 12.505 595 1.00 55.58 MOTA 4521 LEU CB 595 52.619 -11.902 13.020 1.00 54.05 MOTA 4522 CG LEU 595 53.570 -11.074 12.153 1.00 56.23 MOTA 4523 CD1 LEU 595 53.496 -9.609 12.524 1.00 58.84 MOTA 4524 CD2 LEU 595 54.977 -11.596 12.301 1.00 55.93 MOTA 4525 C LEU 595 51.480 -14.093 13.372 1.00 53.77 MOTA 4526 0 LEU 595 50.276 -14.046 13.139 1.00 54.31 MOTA 4527 N SER 596 52.012 -14.780 14.377 1.00 51.04 MOTA 4529 CA SER 51.206 -15.541 15.316 1.00 48.97 596 ATOM 4530 CB SER 596 52.004 -16.737 15.834 1.00 48.89 MOTA 4531 OG SER 596 52.945 -16.345 16.820 1.00 48.59 **ATOM** 4533 С SER 596 50.853 -14.641 16.488 1.00 47.56 MOTA 4534 0 SER 596 51.470 -13.590 16.676 1.00 46.71 **ATOM** 4535 N SER 597 49.888 -15.070 17.292 1.00 47.11 MOTA 4537 CA SER 597 49.462 -14.315 18.461 1.00 47.88 ATOM 4538 CB SER 597 48.386 -15.084 19.229 1.00 50.66 MOTA 4539 OG SER 597 47.574 -15.839 18.343 1.00 57.08 ATOM 4541 50.666 19.372 C SER 597 -14.068 1.00 46.03 **ATOM** 4542 0 SER 597 50.735 -13.045 20.047 1.00 46.49 4543 MOTA N LYS 598 51.607 -15.007 19.399 1.00 46.08 MOTA 52.798 4545 CA LYS 598 -14.844 20.229 1.00 46.33 MOTA 4546 53.558 CB LYS 598 -16.163 20.384 1.00 46.67

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ATOM 4547 CG LYS 598 54.449 -16.224 21.623 1.00 49.61 MOTA 4548 CD LYS 598 55.240 -17.539 21.668 1.00 53.69 **MOTA** 4549 CE LYS 598 55.899 -17.797 23.026 1.00 53.15 MOTA 4550 NZ LYS 598 54.891 -18.076 24.093 1.00 52.02 MOTA 4554 C LYS 598 53.706 -13.790 19.599 1.00 45.43 MOTA 4555 0 LYS 598 54.292 -12.968 20.311 1.00 44.18 MOTA 4556 N ASP 599 53.780 -13.804 18.264 1.00 44.16 **ATOM** 4558 CA ASP 599 54.598 -12.851 17.513 1.00 43.46 MOTA 4559 CB ASP 599 54.523 -13.098 16.001 44.83 1.00 MOTA 4560 CG **ASP** 599 55.288 -14.336 15.560 1.00 48.24 **ATOM** 4561 OD1 **ASP** 599 56.228 -14.754 16.260 1.00 52.90 **ATOM** 4562 OD2 ASP 599 54.958 -14.894 14.493 1.00 51.43 MOTA 4563 C **ASP** 599 54.120 -11.437 17.796 1.00 42.71 --- ATOM 4564 0 ASP 599 54.937 -10.550 18.059 1.00 45.00 ATOM 4565 N LEU 600 52.803 -11.235 17.776 1.00 37.69 MOTA 4567 CA LEU 600 52.246 -9.918 18.030 1.00 34.03 ATOM 4568 CB LEU 600 50.747 -9.882 17.747 1.00 34.06 **ATOM** 4569 CG LEU 600 50.332 -10.068 16.281 1.00 33.13 **ATOM** 4570 CD1 LEU 600 48.814 -9.992 16.190 1.00 37.38 **ATOM** 4571 CD2 LEU 600 50.974 -9.012 15.373 1.00 25.63 **ATOM** 4572 C LEU 600 52.537 -9.452 19.439 1.00 34.58 ATOM 4573 О LEU 600 52.910 -8.294 19.636 1.00 33.18 MOTA 4574 N VAL 601 52.415 -10.348 20.419 1.00 34.24 **MOTA** 4576 CA VAL 601 52.692 -9.969 21.808 1.00 35.80 **ATOM** 4577 CB VAL 601 52.214 -11.036 22.827 1.00 37.50 ATOM 4578 CG1 VAL 601 52.331 -10.483 24.252 1.00 38.08 **MOTA** 4579 CG2 VAL 601 50.766 -11.409 22.560 1.00 40.77 MOTA 4580 С VAL 601 54.198 -9.741 21.982 1.00 35.04 **ATOM** 4581 0 VAL 601 54.634 -8.856 22.731 1.00 34.33 **ATOM** 4582 N SER 602 54.981 -10.531 21.262 1.00 32.58 **ATOM** 4584 CA SER 602 56.421 -10.421 21.307 1.00 36.01 **ATOM** 4585 CB SER 602 57.045 -11.504 20.439 1.00 38.43 MOTA 4586 OG SER 602 58.453 -11.387 20.419 1.00 43.36 MOTA 4588 C SER 602 56.809 -9.038 20.800 1.00 35.21 MOTA 4589 0 SER 602 57.651 -8.363 21.394 1.00 35.03 **ATOM** 4590 N CYS 603 56.183 -8.614 19.707 1.00 34.15 MOTA 4592 CA CYS 603 56.438 -7.294 19.141 1.00 34.04 MOTA 4593 CB CYS 603 55.543 -7.055 17.925 1.00 33.45 MOTA 4594 SG CYS 603 55.653 -5.423 17.229 0.50 32.19 PRT1 MOTA 4595 C CYS 603 56.198 -6.211 20.191 1.00 32.79 MOTA 4596 O CYS 603 57.023 -5.316 20.362 1.00 33.36 **ATOM** 4597 N ALA 604 55.088 -6.321 20.917 1.00 31.31 MOTA 4599 CA ALA 604 54.743 -5.358 21.965 1.00 32.36 **ATOM** 4600 CB ALA 604 53.321 -5.610 22.481 1.00 32.01 MOTA 4601 С ALA 604 55.741 -5.394 23.128 1.00 32.83 **ATOM** 4602 0 ALA 604 56.050 -4.358 23.727 1.00 30.89 **ATOM** 4603 N TYR 605 56.212 -6.592 23.465 1.00 32.95 **ATOM** 4605 CA TYR 605 57.189 -6.758 24.539 1.00 33.34 **ATOM** 4606 CB TYR 605 57.500 -8.236 24.737 1.00 32.58 MOTA 4607 CG TYR 605 58.640 -8.495 25.690 1.00 32.51 MOTA 4608 CD1 TYR 605 58.511 -8.236 27.053 1.00 33.50 **ATOM** 4609 CEl TYR 605 59.556 -8.507 27.943 1.00 37.08 **ATOM** 4610 CD2 TYR 605 59.841 -9.026 25.230 1.00 34.22 **ATOM** CE2 4611 TYR 605 60.896 -9.300 26.109 1.00 36.64

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-9.042 27.464 1.00 37.56 **ATOM** 4612 CZ TYR 605 60.746 ATOM 4613 605 61.776 -9.342 28.336 1.00 38.08 OH TYR -6.006 MOTA 58.480 24.191 1.00 32.42 4615 C TYR 605 MOTA 4616 58.975 -5.203 24.991 1.00 33.34 0 TYR 605 MOTA 4617 N GLN 606 58.997 -6.267 22.989 1.00 30.61 MOTA 4619 60.218 -5.643 22.474 CA GLN 606 1.00 31.12 ATOM 4620 CB GLN 606 60.499 -6.143 21.058 1.00 30.57 MOTA 4621 CG GLN 606 61.044 -7.568 21.008 1.00 33.90 MOTA -8.080 4622 CD GLN 606 61.240 19.593 1.00 32.17 ATOM 4623 OE1 GLN 606 62.155 **-7.6**52 18.883 1.00 32.55 MOTA 60.374 -8.998 4624 NE₂ GLN 606 19.171 1.00 33.10 **ATOM** 4627 \mathbf{c} GLN 606 60.157 -4.114 22.487 1.00 31.69 **ATOM** 4628 o GLN 606 61.111 -3.453 22.910 1.00 31.18 MOTA 4629 N VAL 607 59.035 -3.564 22.020 1.00 .. 29.50.... MOTA 4631 CA VAL 607 58.816 -2.122 22.000 1.00 27.54 MOTA 4632 CB VAL 607 57.454 -1.751 21.306 1.00 26.79 **ATOM** 4633 CG1 VAL 607 57.131 -0.291 21.516 1.00 24.80 MOTA -2.050 4634 CG2 VAL 607 57.505 19.815 1.00 22.95 MOTA 4635 C VAL 607 58.827 -1.576 23.432 1.00 28.30 MOTA 607 -0.548 4636 0 VAL 59.469 23.705 1.00 28.32 MOTA 608 4637 N ALA 58.110 -2.247 24.340 1.00 27.21 ATOM 4639 CA ALA 608 58.061 -1.805 25.735 1.00 26.54 ATOM CB 608 4640 ALA 57.070 -2.649 26.550 1.00 26.70 ATOM 4641 C ALA 608 59.457 -1.850 26.368 1.00 25.97 MOTA 4642 0 ALA 608 59.802 -0.993 27.183 1.00 25.88 **ATOM** 4643 N ARG 609 60.250 -2.848 25.994 1.00 26.02 **MOTA** 4645 CA ARG 609 61.606 -2.977 26.512 1.00 30.44 ATOM 4646 CR ARG 609 62.234 -4.285 26.058 1.00 34.09 **ATOM** 4647 CG ARG 609 61.642 -5.516 26.682 1.00 39.24 MOTA 4648 CD ARG 609 62.659 -6.615 26.615 1.00 42.75 ATOM 4649 NE ARG 609 63.405 -6.704 27.860 1.00 45.52 MOTA 609 -7.405 4651 CZARG 64.525 28.019 1.00 46.24 MOTA 4652 NH1 ARG 609 65.055 -8.079 27.001 1.00 41.48 ATOM 4655 NH2 ARG 609 65.079 -7.482 29.225 1.00 47.49 ATOM 4658 C ARG 609 62.478 -1.82926.015 1.00 34.20 MOTA 4659 0 ARG 609 63.265 -1.255 26.788 1.00 35.24 ATOM 4660 GLY 610 62.368 -1.528 24.717 1.00 N 33.25 MOTA 4662 CA GLY 610 63.130 -0.439 24.138 1.00 29.57 ATOM 4663 C GLY 610 62.802 0.814 24.908 1.00 29.31 **ATOM** 4664 GLY 63.695 1.543 0 610 25.335 1.00 27.46 MOTA 4665 N MET 611 61.507 1.020 25.147 1.00 31.07 MOTA 4667 CA MET 611 61.016 2.178 25.889 1.00 30.09 **ATOM** 4668 CB MET 611 59.493 2.280 25.782 1.00 29.51 MOTA 4669 CG MET 611 58.997 2.655 24.404 1.00 28.21 MOTA 4670 SD MET 611 59.760 4.175 23.787 1.00 29.00 MOTA 4671 CE MET 611 59.350 5.335 25.039 1.00 25.91 MOTA 4672 С MET 611 61.439 2.189 27.361 1.00 30.47 MOTA 4673 0 MET 611 61.734 3.242 27.919 1.00 29.43 **ATOM** 4674 N GLU 612 61.429 1.031 28.002 1.00 31.97 ATOM 4676 CA GLU 612 61.836 0.947 29.402 1.00 35.34 ATOM 4677 CB GLU 612 61.707 ~0.490 29.904 1.00 36.17 MOTA 4678 CG GLU 612 62.305 -0.729 31.278 1.00 34.87 **ATOM** 4679 CD GLU 612 62.259 -2.185 31.705 1.00 32.68 MOTA 4680 OE1 GLU 612 62.641 -3.070 30.904 1.00 35.01

ATOM 4681 OE₂ GLU 612 61.848 32.858 -2.443 1.00 36.56 **ATOM** 4682 C GLU 612 63.296 1.425 29.490 1.00 35.26 **ATOM** 4683 0 GLU 612 63.677 2.162 30.417 1.00 31.21 MOTA 4684 N TYR 613 64.092 1.040 28.491 1.00 36.10 MOTA 4686 CA TYR 613 65.491 1.458 28.440 1.00 34.76 MOTA 4687 CB TYR 613 66.249 0.788 27.301 1.00 31.15 MOTA 4688 CG TYR 613 67.700 1.195 27.284 1.00 34.28 **ATOM** 4689 CD1 TYR 613 68.600 0.654 28.207 1.00 36.50 MOTA 4690 CEl TYR 613 69.949 1.035 28.219 1.00 38.20 MOTA 4691 CD2 TYR 613 68.179 2.135 26.366 1.00 32.99 MOTA 4692 CE2 TYR 613 69.520 2.526 26.372 1.00 33.32 MOTA 4693 CZTYR 613 70.399 1.968 27.302 1.00 36.59 MOTA 4694 OH TYR 613 71.721 2.340 27.333 1.00 35.73 MOTA - 4696 C. - - -TYR -- 613--28.273 65.583 2.970 1.00 34.03 and the specific factors of the second ATOM 4697 0 TYR 613 66.231 3.643 29.075 1.00 35.26 **ATOM** 4698 N LEU 614 64.916 3.503 27.250 1.00 31.78 **ATOM** 4700 CA LEU 614 64.945 4.937 26.998 1.00 29.50 **ATOM** 4701 CB LEU 614 64.095 5.297 25.775 1.00 28.26 ATOM 4702 CG LEU 614 64.564 4.742 24.422 1.00 31.29 CD1 MOTA 4703 LEU 614 63.564 5.089 23.321 1.00 28.09 ATOM 4704 CD2 LEU 614 65.951 5.282 24.079 29.52 1.00 MOTA 4705 C LEU 614 64.489 5.715 28.224 1.00 32.49 **ATOM** 4706 О LEU 614 65.108 6.717 28.598 1.00 31.73 MOTA 4707 N ALA 615 63.431 5.232 28.872 1.00 33.06 **ATOM** 4709 CA ALA 615 62.906 5.870 30.070 1.00 35.16 **MOTA** 4710 CB ALA 615 61.598 5.192 30.511 1.00 36.64 **ATOM** 4711 C ALA 615 63.942 5.838 31.202 1.00 35.36 MOTA 4712 O ALA 615 64.065 6.805 31.952 1.00 36.80 MOTA 4713 N SER 616 64.690 4.739 31.315 1.00 35.91 **ATOM** 4715 CA SER 616 65.716 4.621 32.354 1.00 35.78 **ATOM** 4716 SER CB 616 66.287 3.199 32.424 1.00 32.52 MOTA 4717 OG SER 616 67.133 2.899 31.324 1.00 29.64 MOTA 4719 C SER 616 66.832 5.623 32.063 1.00 37.48 MOTA 4720 0 SER 616 67.556 6.048 32.967 1.00 38.76 MOTA 4721 N LYS 617 66.971 5.980 30.790 1.00 34.74 MOTA 4723 CA LYS 617 67.973 6.931 30.357 1.00 32.44 MOTA 4724 CB LYS 617 68.540 28.998 6.520 1.00 32.94 MOTA 4725 CG LYS 617 69.330 5.232 29.041 1.00 32.64 MOTA 4726 CD LYS 617 70.539 5.402 29.933 1.00 38.45 MOTA 4727 CE LYS 617 71.252 4.091 30.139 1.00 40.84 MOTA 4728 NZ LYS 617 72.552 4.306 30.812 1.00 46.49 MOTA 4732 C LYS 617 67.376 8.325 30.281 1.00 33.29 MOTA 4733 O LYS 617 67.909 9.188 29.598 1.00 33.95 MOTA 4734 N LYS 618 66.245 8.528 30.952 1.00 34.87 MOTA 4736 CA LYS 618 65.569 9.822 30.997 1.00 35.44 MOTA 4737 66.512 CB LYS 618 10.868 31.581 1.00 40.44 MOTA 4738 CG LYS 618 67.192 10.446 32.877 1.00 48.19 MOTA 4739 CD LYS 618 66.234 10.363 34.037 1.00 55.47 MOTA 4740 CE LYS 618 9.939 66.962 35.310 1.00 61.56 **ATOM** 4741 NZ LYS 618 66.070 10.032 36.514 1.00 68.82 MOTA 4745 C LYS 618 65.015 10.327 29.663 1.00 35.62 ATOM 4746 0 LYS 618 64.557 11.463 29.569 1.00 36.44 ATOM 4747 619 N CYS 65.006 9.472 28.647 1.00 34.24 **ATOM** 4749 CA CYS 619 64.525 9.848 27.323 1.00 31.62

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ATOM 4750 CB CYS 619 65.279 9.033 26.263 1.00 31.17 MOTA 4751 SG CYS 619 64.816 9.306 24.541 1.00 30.02 **ATOM** 4752 С CYS 619 63.004 9.701 27.149 1.00 30.45 **ATOM** 4753 0 CYS 619 62.418 8.649 27.388 1.00 29.24 MOTA 4754 N ILE 620 62.359 10.798 26.800 1.00 30.14 MOTA 4756 CA ILE 620 60.935 10.822 26.542 1.00 31.76 ATOM 4757 CB ILE 620 60.268 12.040 27.193 1.00 31.26 26.774 MOTA 4758 CG2 ILE 620 58.799 12.116 1.00 31.66 MOTA 4759 CG1 ILE 620 60.392 11.957 28.712 1.00 29.71 ATOM 4760 CDI ILE 620 60.016 13.236 29.396 1.00 27.40 MOTA 4761 С ILE 620 60.864 10.961 25.023 1.00 31.86 ATOM 4762 0 ILE 620 61.384 11.920 24.465 1.00 32.70 MOTA ,4763 N HIS 621 60.249 9.986 24.366 1.00 31.70 __60.133 MOTA 4765 CA HIS 621 9.973 22.906 1.00 32.12 MOTA 4766 CB HIS 621 59.708 8.578 22.430 1.00 29.61 MOTA 4767 CG HIS 621 59.903 8.344 20.961 1.00 28.62 MOTA 4768 CD2 HIS 621 60.511 7.336 20.300 1.00 27.49 **ATOM** 4769 ND1 HIS 621 59.373 9.168 19.988 1.00 30.08 **ATOM** 4771 CE1 HIS 621 59.637 8.669 18.795 1.00 25.00 MOTA 4772 NE₂ HIS 621 60.325 7.554 18.956 1.00 26.55 MOTA 4774 C HIS 621 59.194 11.026 22.321 1.00 34.51 MOTA 4775 O HIS 621 59.466 11.570 21.251 1.00 36.79 MOTA 4776 N ARG 622 58.048 11.248 22.960 1.00 35.26 MOTA 4778 CA ARG 622 57.068 12.239 22.490 1.00 34.68 ATOM 4779 CB ARG 622 57.705 13.628 22.370 1.00 33.43 MOTA 4780 CG ARG 622 58.285 14.135 23.674 1.00 31.52 MOTA 4781 CD ARG 622 58.781 15.563 23.570 0.50 27.82 MOTA 4782 NE ARG 622 59.216 16.050 24.876 0.50 28.82 MOTA 4784 CZ ARG 622 60.362 15.715 25.463 0.50 30.41 MOTA 4785 NH1 ARG 622 61.215 14.891 24.860 0.50 31.15 MOTA 4788 NH2 ARG 622 60.640 16.168 26.680 0.50 30.83 MOTA 4791 C ARG 622 56.283 11.891 21.213 1.00 34.71 MOTA 4792 0 ARG 622 55.289 12.544 20.912 1.00 35.58 MOTA 4793 N ASP 623 56.719 10.884 20.459 1.00 34.90 MOTA 4795 CA ASP 623 55.986 10.468 19.261 1.00 34.30 ATOM 4796 CB ASP 623 56.443 11.212 17.994 1.00 36.76 ATOM 4797 CG ASP 623 55.535 10.918 16.772 1.00 43.35 MOTA 4798 OD1 **ASP** 623 55.980 11.131 1.00 15.624 47.64 MOTA 4799 OD2 **ASP** 623 54.376 10.469 16.954 1.00 43.30 MOTA 4800 С ASP 623 56.094 8.967 19.051 1.00 32.24 ATOM 4801 0 ASP 623 56.406 8.494 17.957 1.00 31.19 MOTA 4802 N LEU 624 55.895 8.209 20.118 1.00 32.27 MOTA 4804 CA LEU 624 55.964 6.759 20.005 1.00 33.18 MOTA 4805 CB LEU 624 56.013 6.118 21.390 1.00 31.16 **MOTA** 4806 CG LEU 624 56.019 4.592 21.452 1.00 32.74 MOTA 4807 CD1 LEU 624 57.257 4.020 20.765 1.00 30.64 MOTA 4808 CD2 LEU 624 55.974 4.177 22.904 1.00 34.51 ATOM 4809 C LEU 624 54.738 6.274 19.217 1.00 35.18 **ATOM** 4810 0 LEU 624 53.589 6.511 19.612 1.00 35.72 MOTA 4811 N ALA 625 54.997 5.632 18.084 1.00 32.37 MOTA 4813 CA ALA 625 53.946 5.113 17.223 1.00 30.60 MOTA 4814 CB 625 ALA 53.447 6.205 16.298 1.00 25.26 MOTA 4815 С ALA 625 54.618 4.020 16.427 1.00 29.87 ATOM 4816 0 ALA 625 55.839 3.978 16.378 1.00 32.01

ATOM	4817	N	ALA	626	53.834	3.163	15.779	1.00	30.12
ATOM	4819	CA	ALA	626	54.373	2.057	14.978	1.00	29.62
MOTA	4820	CB	ALA	626	53.231	1.159	14.441	1.00	27.11
ATOM	4821	C	ALA	626	55.255	2.552	13.838	1.00	26.57
MOTA	4822	0	ALA	626	56.193	1.871	13.434	1.00	26.29
MOTA	4823	N	ARG	627	54.935	3.730	13.317	1.00	26.74
ATOM	4825	CA	ARG	627	55.706	4.352	12.244	1.00	28.73
MOTA	4826	CB	ARG	627	55.056	5.671	11.827	1.00	29.62
MOTA	4827	CG	ARG	627	54.894	6.659	12.972	1.00	31.84
MOTA	4828	CD	ARG	627	54.435	8.032	12.485	1.00	38.54
MOTA	4829	NE	ARG	627	53.987	8.878	13.590	1.00	38.59
ATOM	4831	CZ	ARG	627	52.745	8.879	14.064	1.00	39.55
MOTA	4832	NH1	ARG	627	51.822	8.094	13.525	1.00	35.96
ATOM	4835	NH2	ARG	627	52.447	9.604	15.127	1.00	41.05
ATOM	4838	С	ARG	627	57.151	4.632	12.676	1.00	30.79
MOTA	4839	0	ARG	627	58.058	4.687	11.838	1.00	30.16
ATOM	4840	N	ASN	628	57.347	4.822	13.985	1.00	30.31
MOTA	4842	CA	asn	628	58.661	5.109	14.550	1.00	28.50
ATOM	4843	CB	ASN	628	58.587	6.257	15.549	1.00	27.84
ATOM	4844	CG	ASN	628	58.369	7.571	14.868	1.00	31.41
ATOM	4845	OD1	ASN	628	58.893	7.796	13.782	1.00	33.45
ATOM	4846	ND2	ASN	628	57.551	8.429	15.460	1.00	28.53
MOTA	4849	С	ASN	628	59.352	3.919	15.169	1.00	28.10
ATOM	4850	0	ASN	628	60.232	4.076	16.021	1.00	28.64
ATOM	4851	N	VAL	629	58.887	2.733	14.803	1.00	27.79
ATOM	4853	CA	VAL	629	59.484	1.482	15.253	1.00	28.30
ATOM	4854	CB	VAL	629	58.475	0.577	15.983	1.00	25.38
ATOM ATOM	4855	CG1	VAL	629	59.118	-0.753	16.284	1.00	23.07
ATOM	4856 4857	CG2 C	VAL VAL	629 629	57.980	1.246	17.265	1.00	22.48
ATOM	4858	0	VAL	629	59.925 59.114	0.810	13.949	1.00	28.69
ATOM	4859	N	LEU	630	61.220	0.616 0.542	13.043 13.823	1.00	27.07
ATOM	4861	CA	LEU	630	61.749	-0.081	12.616	1.00	29.54 30.17
ATOM	4862	СВ	LEU	630	62.999	0.659	12.142	1.00	29.62
ATOM	4863	CG	LEU	630	62.831	2.180	12.035	1.00	29.14
MOTA	4864	CD1	LEU	630	64.121	2.795	11.579	1.00	29.83
ATOM	4865	CD2	LEU	630	61.693	2.543	11.086	1.00	32.59
ATOM	4866	C	LEU	630	62.036	-1.541	12.899	1.00	30.50
MOTA	4867	0	LEU	630	62.290	-1.910	14.042	1.00	31.06
MOTA	4868	N	VAL	631	61.966	-2.376	11.866	1.00	33.03
ATOM	4870	CA	VAL	631	62.174	-3.813	12.022	1.00	31.83
MOTA	4871	СВ	VAL	631	60.902	-4.605	11.582	1.00	29.48
ATOM	4872	CG1	VAL	631	61.017	-6.067	11.980	1.00	29.39
ATOM	4873	CG2	VAL	631	59.644	-3.984	12.196	1.00	25.38
ATOM	4874	C	VAL	631	63.379	-4.242	11.196	1.00	32.37
MOTA	4875	0	VAL	631	63.508	-3.865	10.024	1.00	33.57
ATOM	4876	N	THR	632	64.285	-4.987	11.820	1.00	34.39
ATOM	4878	CA	THR	632	65.504	-5.453	11.145	1.00	35.84
ATOM	4879	CB	THR	632	66.659	-5.685	12.148	1.00	33.11
ATOM	4880	OG1	THR	632	66.328	-6.774	13.020	1.00	34.88
ATOM	4882	CG2	THR	632	66.922	-4.426	12.972	1.00	28.85
ATOM	4883	С	THR	632	65.272	-6.738	10.350	1.00	37.63
ATOM	4884	0	THR	632	64.195	-7.347	10.439	1.00	37.20
MOTA	4885	N	GLU	633	66.289	-7.163	9.600	1.00	39.78

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MOTA 4887 8.794 CA GLU 66.182 1.00 633 -8.379 43.30 **ATOM** 4888 CB 67.437 1.00 GLU 633 -8.590 7.933 46.66 51.37 MOTA 4889 CG GLU 633 67.336 -9.729 6.876 1.00 **ATOM** 4890 CD 1.00 **GLU** 633 66.490 -9.404 5.622 54.30 ATOM 4891 OE1 GLU 633 1.00 65.859 -8.327 5.523 55.85 MOTA 4892 OE2 GLU 633 4.710 1.00 66.460 -10.256 55.95 MOTA 4893 С GLU 633 65.919 -9.592 9.677 1.00 42.72 MOTA 4894 0 GLU 633 65.360 -10.582 9.222 1.00 45.10 ATOM 4895 N **ASP** 634 66.287 -9.494 10.949 1.00 42.83 MOTA 4897 CA ASP 634 66.075 -10.585 11.884 1.00 43.03 ATOM 4898 CB ASP 634 67.324 -10.809 12.743 1.00 49.02 MOTA 4899 CG ASP 634 68.539 -11.240 11.916 1.00 55.95 **ATOM** 4900 OD1 ASP 634 68.462 -12.292 11.237 1.00 59.10 ATOM 4901 OD2 ASP 634 69.568 -10.525 11.943 1.00 59.41 **ATOM** 4902 C ASP 634 64.848 -10.340 12.751 1.00 41.75 **ATOM** 4903 0 ASP 64.737 -10.873 1.00 634 13.847 42.79 ATOM 4904 N ASN 635 63.937 -9.508 12.257 1.00 42.51 MOTA 4906 CA ASN 635 62.686 -9.186 12.939 1.00 42.53 MOTA 4907 CB ASN 635 61.768 -10.417 12.992 1.00 45.07 **ATOM** 4908 CG ASN 635 61.483 -10.985 11.624 1.00 46.54 MOTA 4909 OD1 ASN 635 60.868 -10.336 10.786 1.00 49.77 **MOTA** 4910 ND2 ASN 635 61.949 -12.192 11.383 1.00 49.29 **ATOM** 4913 C ASN 635 62.801 -8.577 1.00 14.331 40.51 **ATOM** 4914 O ASN 635 61.939 -8.800 15.187 1.00 41.80 ATOM 4915 N VAL 636 63.844 -7.795 14.561 1.00 37.98 MOTA 4917 CA VAL 636 64.016 -7.164 15.856 1.00 33.92 MOTA 4918 CB VAL 636 65.517 -7.005 16.195 1.00 32.21 MOTA 4919 VAL CG1 636 65.697 -6.284 17.530 1.00 31.40 MOTA 4920 CG2 VAL 636 66.169 -8.367 16.242 1.00 30.93 MOTA 4921 С VAL 636 63.349 -5.797 15.811 1.00 31.85 **ATOM** 4922 0 VAL 636 63.531 -5.061 14.849 1.00 33.47 MOTA 4923 N MET 637 -5.492 62.525 16.807 1.00 31.69 MOTA 4925 CA MET 637 61.860 -4.194 16.879 1.00 31.44 MOTA 4926 CB MET 637 60.642 -4.241 17.820 1.00 34.97 MOTA 4927 CG MET 637 59.559 -5.264 17.455 1.00 36.80 MOTA 4928 SD MET 637 58.860 -5.048 15.803 1.00 35.45 MOTA 4929 CE MET 637 59.030 -6.709 15.116 1.00 32.12 MOTA 4930 С MET 637 62.874 -3.209 17.454 1.00 31.86 MOTA 4931 0 MET 637 63.512 -3.496 18.479 1.00 29.47 MOTA 4932 N 638 LYS 62.985 -2.041 16.820 1.00 30.87 MOTA 4934 CA LYS 638 63.915 -0.994 17.244 1.00 29.66 СВ MOTA 4935 LYS 638 65.161 -0.983 16.349 1.00 27.51 MOTA 4936 CG LYS 638 66.171 -2.059 16.691 1.00 27.29 MOTA 4937 CD LYS 638 67.370 -1.984 15.781 1.00 28.55 ATOM 4938 CE LYS 638 68.409 -3.029 16.150 1.00 24.75 ATOM 4939 NZ 638 25.59 LYS 68.964 -2.785 17.498 1.00 ATOM 4943 C LYS 638 63.283 0.383 17.215 1.00 27.72 MOTA 4944 O LYS 638 62.918 0.869 16.146 1.00 27.66 MOTA 4945 N ILE 639 63.163 1.004 18.387 1.00 26.21 MOTA 4947 CA ILE 639 62.597 2.343 18.501 1.00 26.27 MOTA 4948 CB ILE 639 62.580 2.862 19.965 1.00 26.52 MOTA 4949 CG2 ILE 639 61.896 4.206 20.017 1.00 21.50 ATOM 4950 CG1 ILE 639 61.918 1.854 20.926 1.00 25.70 ATOM 4951 CD1 ILE 639 60.496 1.494 20.599 1.00 25.62

ATOM	4952	C	ILE	639	63.50 5	3.288	17.718	1.00	29.56
ATOM	4953	0	ILE	639	64.730	3.281	17.906	1.00	27.74
ATOM	4954	N	ALA	640	62.897	4.101	16.857	1.00	27.91
ATOM	4956	CA	ALA	640	63.620	5.071	16.042	1.00	28.79
MOTA	4957	CB	ALA	640	63.377	4.796	14.563	1.00	26.74
MOTA	4958	С	ALA	640	63.164	6.487	16.385	1.00	28.91
MOTA	4959	0	ALA	640	62.087	6.683	16.956	1.00	28.67
MOTA	4960	N	ASP	641	64.007	7.464	16.067	1.00	28.25
MOTA	4962	CA	ASP	641	63.708	8.876	16.296	1.00	30.80
ATOM	4963	CB	ASP	641	62.520	9.319	15.428	1.00	33.44
MOTA	4964	CG	ASP	641	62.869	9.393	13.948	1.00	38.01
MOTA	4965	OD1	ASP	641	64.002	9.001	13.574	1.00	42.41
MOTA	4966	OD2	ASP	641	62.006	9.847	13.160	1.00	41.74
MOTA	4967	C.	ASP	641	63.501	9.311	17.745	1:00	29::07
MOTA	4968	0	ASP	641	62.847	10.309	18.020	1.00	28.42
MOTA	4969	N	PHE	642	64.138	8.604	18.663	1.00	29.69
ATOM	4971	CA	PHE	642	64.036	8.914	20.074	1.00	29.62
MOTA	4972	CB	PHE	642	64.347	7.656	20.890	1.00	27.18
MOTA	4973	CG	PHE	642	65.702	7.058	20.603	1.00	23.96
ATOM	4974	CD1	PHE	642	66.848	7.559	21.219	1.00	23.66
ATOM	4975	CD2	PHE	642	65.828	5.974	19.742	1.00	24.08
MOTA	4976	CE1	PHE	642	68.090	6.992	20.980	1.00	23.02
ATOM	4977	CE2	PHE	642	67.069	5.403	19.501	1.00	23.20
ATOM	4978	CZ	PHE	642	68.200	5.909	20.121	1.00	21.68
ATOM	4979	С	PHE	642	64.948	10.075	20.502	1.00	32.99
ATOM	4980	0	PHE	642	64.755	10.664	21.574	1.00	32.10
ATOM	4981	N	GLY	643	65.940	10.396	19.671	1.00	34.66
ATOM	4983	CA	GLY	643	66.869	11.463	20.003	1.00	35.29
MOTA	4984	С	GLY	643	66.639	12.755	19.250	1.00	39.13
MOTA	4985	0	GLY	643	67.464	13.666	19.333	1.00	39.83
MOTA	4986	N	LEU	644	65.520	12.850	18.532	1.00	42.26
MOTA	4988	CA	LEU	644	65.202	14.043	17.745	1.00	46.25
ATOM	4989	CB	LEU	644	63.935	13.843	16.911	1.00	44.59
ATOM	4990	CG	LEU	644	63.911	12.839	15.763	1.00	43.00
ATOM	4991	CD1	LEU	644	62.653	13.068	14.940	1.00	42.61
ATOM	4992	CD2	LEU	644	65.119	13.016	14.889	1.00	45.65
MOTA	4993	С	LEU	644	65.037	15.298	18.578	1.00	49.59
MOTA	4994	0	LEU	644	64.391	15.281	19.623	1.00	51.90
MOTA	4995	N	ALA	645	65.585	16.401	18.080	1.00	52.08
MOTA	4997	CA	ALA	645	65.495	17.677	18.777	1.00	54.71
MOTA	4998	CB	ALA	645	66.414	18.699	18.124	1.00	54.38
MOTA	4999	C	ALA	645	64.053	18.184	18.790	1.00	55.44
MOTA	5000	0	ALA	645	63.534	18.582	19.832	1.00	56.69
MOTA	5001	N	ASP	652	52.389	21.543	14.759	1.00	73.74
MOTA	5003	CA	ASP	652	51.207	21.745	13.934	1.00	73.83
MOTA	5004	CB	ASP	652	51.601	21.995	12.472	1.00	73.22
ATOM	5005	CG	ASP	652	50.398	22.241	11.569	1.00	72.95
ATOM	5006	OD1	ASP	652	49.354	22.715	12.065	1.00	73.71
MOTA	5007	OD2	ASP	652	50.497	21.956	10.357	1.00	73.02
ATOM	5008	С	ASP	652	50.321	20.514	14.042	1.00	75.11
ATOM	5009	0	ASP	652	50.568	19.495	13.394	1.00	75.96
ATOM	5010	N	TYR	653	49.272	20.628	14.849	1.00	75.57
ATOM	5012	CA	TYR	653	48.348	19.524	15.064	1.00	75.68
ATOM	5013	СВ	TYR	653	47.274	19.914	16.088	1.00	76.85

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1.00 **ATOM** 19.995 17.519 79.55 5014 CG TYR 653 47.771 **ATOM** 20.567 18.518 1.00 80.89 5015 CD1 TYR 653 46.983 MOTA 5016 CE1 TYR 653 47.438 20.648 19.836 1.00 83.02 **MOTA** 5017 CD2 49.032 19.503 1.00 80.87 TYR 653 17.874 ATOM 5018 CE2 TYR 653 49.496 19.578 19.183 1.00 81.70 MOTA 5019 CZ TYR 653 48.698 20.152 20.160 1.00 83.09 MOTA 5020 OH TYR 653 49.165 20.243 21.451 1.00 83.73 MOTA 5022 С TYR 653 47.685 19.038 13.787 1.00 75.03 MOTA 5023 0 TYR 653 47.232 17.897 13.711 1.00 75.97 **ATOM** 5024 N TYR 654 47.679 19.885 12.767 1.00 73.85 MOTA 5026 CA TYR 654 47.039 19.538 11.507 1.00 73.32 MOTA 5027 CB TYR 654 46.276 20.750 10.972 1.00 71.97 MOTA 5028 CG TYR 654 45.259 21.276 11.954 1.00 70.94 MOTA 1.00 71.41 5029 CD1 TYR 654 45.659 21.801 13.185 MOTA 5030 CE1 TYR 654 44.733 22,234 14.121 1.00 73.60 MOTA 5031 CD2 TYR 654 43.899 21.206 11.680 1.00 71.81 MOTA 5032 CE2 TYR 654 42.956 21.642 12.610 1.00 74.81 MOTA 5033 CZ654 TYR 43.380 22.152 13.832 1.00 74.84 MOTA 5034 OH TYR 654 42.457 22.571 14.769 1.00 76.60 MOTA 5036 С TYR 654 47.975 18.967 10.446 1.00 73.82 9.329 MOTA 5037 0 TYR 654 47.545 18.671 1.00 74.25 MOTA 5038 655 N LYS 49.249 18.806 10.784 1.00 74.04 MOTA 5040 CA LYS 655 50.195 18.256 9.827 1.00 75.41 MOTA 5041 CB LYS 655 51.626 18.680 10.164 1.00 78.45 **ATOM** 5042 CG LYS 655 52.647 18.198 9.151 1.00 83.01 **MOTA** 5043 87.72 CD LYS 655 54.062 18.589 9.537 1.00 MOTA 5044 CE LYS 655 55.076 17.813 8.703 1.00 91.45 MOTA 5045 NZ LYS 655 56.489 18.133 9.074 1.00 94.17 MOTA 5049 С LYS 655 50.075 16.736 9.832 1.00 75.50 MOTA 5050 LYS 655 10.872 1.00 0 50.245 16.092 75.90 **MOTA** 5051 N LYS 656 49.750 16.173 8.672 1.00 75.26 MOTA 5053 CA LYS 656 49.597 14.730 8.533 1.00 74.97 MOTA 5054 CB LYS 656 48.723 14.406 7.323 1.00 75.40 MOTA 5055 CG LYS 656 47.266 14.753 7.519 1.00 76.87 MOTA 5056 CD LYS 656 46.489 14.535 6.239 1.00 80.75 MOTA 5057 CE LYS 656 45.001 14.655 6.483 1.00 83.60 **ATOM** 5058 NZ LYS 656 44.236 14.637 5.204 1.00 87.14 MOTA 5062 LYS 656 50.939 14.016 8.414 1.00 C 74.58 MOTA 5063 14.578 0 LYS 656 51.904 7.897 1.00 75.01 MOTA 5064 N GLY 660 49.137 9.764 5.736 1.00 59.18 MOTA 5066 CA GLY 660 48.106 10.781 56.19 5.848 1.00 MOTA 5067 С GLY 660 47.407 10.761 7.192 1.00 55.31 MOTA 5068 0 GLY 660 46.289 7.328 11.263 1.00 56.96 MOTA 5069 N ARG 661 48.059 10.163 B.183 1.00 53.02 **ATOM** 5071 .CA ARG 661 47.493 10.083 9.527 1.00 49.80 MOTA 5072 CB ARG 661 47.944 8.799 10.229 1.00 51.79 MOTA 5073 CG 47.683 ARG 661 7.523 9.450 1.00 50.59 MOTA 5074 CD ARG 661 47.822 6.323 10.367 1.00 53.68 ATOM 5075 NE ARG 661 47.714 5.044 9.665 1.00 52.66 MOTA 5077 CZARG 661 47.928 3.863 10.236 1.00 51.73 MOTA 5078 NH1 ARG 661 48.264 3.794 11.518 1.00 50.23 MOTA 5081 NH2 ARG 661 47.800 2.751 9.528 1.00 52.58 MOTA 5084 C ARG 661 47.915 1.00 11.297 10.346 44.80 MOTA 5085 0 ARG 661 48.865 11.998 9.986 1.00 43.61

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MOTA	5086	N	LEU	662	47.221	11.528	11.453	1.00	40.74
ATOM	5088	CA	LEU	662	47.518	12.654	12.333	1.00	37.88
ATOM	5089	CB	LEU	662	46.234	13.415	12.671	1.00	36.19
ATOM	5090	CG	LEU	662	45.515	14.074	11.499	1.00	35.32
ATOM	5091	CD1	LEU	662	44.045	14.278	11.831	1.00	
ATOM	5092	CD2	LEU	662	46.217	15.383			31.05
ATOM	5093	C	LEU	662	48.162		11.156	1.00	34.37
ATOM	5094	ō	LEU	662		12.170	13.622	1.00	35.34
ATOM	5095	N	PRO	663	47.529	11.479	14.417	1.00	33.06
ATOM	5096				49.441	12.518	13.843	1.00	36.39
		CD	PRO	663	50.375	13.113	12.868	1.00	37.57
MOTA	5097	CA	PRO	663	50.158	12.107	15.054	1.00	36.39
MOTA	5098	CB	PRO	663	51.516	12.787	14.885	1.00	36.98
	5099	CG	PRO	663	51.728	12.657	13.401	1.00	38.48
ATOM	5100	C	PRO	663	49.477	12.491	16.371	1.00	35.47
ATOM	5101	0	PRO	663	49.699	11.841	17.392	1.00	35.08
ATOM	5102	N	VAL	664	48.646	13.532	16.362	1.00	34.28
ATOM	5104	CA	VAL	664	47.951	13.931	17.583	1.00	34.43
ATOM	5105	CB	VAL	664	47.038	15.181	17.376	1.00	36.92
ATOM	5106	CG1	VAL	664	47.885	16.408	17.160	1.00	37.55
MOTA	5107	CG2	VAL	664	46.091	14.989	16.186	1.00	38.28
ATOM	5108	С	VAL	664	47.137	12.749	18.120	1.00	33.03
MOTA	5109	0	VAL	664	46.908	12.641	19.318	1.00	34.62
ATOM	5110	N	LYS	665	46.803	11.809	17.236	1.00	32.47
ATOM	5112	CA	LYS	665	46.040	10.631	17.614	1.00	30.71
ATOM	5113	CB	LYS	665	45.456	9.958	16.370	1.00	29.59
ATOM	5114	CG	LYS	665	44.324	10.774	15.768	1.00	29.64
MOTA	5115	CD	LYS	665	43.927	10.334	14.367	1.00	31.86
MOTA	5116	CE	LYS	665	42.664	11.056	13.899	1.00	30.42
MOTA	5117	NZ	LYS	665	42.296	10.720	12.486	1.00	26.50
ATOM	5121	С	LYS	665	46.801	9.644	18.498	1.00	32.23
MOTA	5122	0	LYS	665	46.230	8.659	18.955	1.00	30.04
ATOM	5123	N	TRP	666	48.080	9.915	18.748	1.00	31.38
ATOM	5125	CA	TRP	666	48.886	9.068	19.619	1.00	32.32
MOTA	5126	CB	TRP	666	50.204	8.682	18.945	1.00	31.07
MOTA	5127	CG	TRP	666	50.078	7.530	18.006	1.00	28.26
MOTA	5128	CD2	TRP	666	49.531	7.559	16.684	1.00	27.07
MOTA	5129	CE2	TRP	666	49.630	6.257	16.163	1.00	26.71
MOTA	5130	CE3	TRP	666	48.982	8.569	15.882	1.00	26.56
ATOM	5131	CD1	TRP	666	50.473	6.238	18.234	1.00	24.97
ATOM	5132	NE1	TRP	666	50.206	5.469	17.132	1.00	27.38
ATOM	5134	CZ2	TRP	666	49.190	5.929	14.874	1.00	27.22
ATOM	5135	CZ3	TRP	666	48.548	8.248	14.599	1.00	30.14
MOTA	5136	CH2	TRP	666	48.658	6.934	14.107	1.00	26.64
ATOM	5137	С	TRP	666	49.203	9.802	20.913	1.00	33.84
MOTA	5138	0	TRP	666	49.688	9.202	21.873	1.00	32.82
ATOM	5139	N	MET	667	48.905	11.099	20.929	1.00	35.75
ATOM	5141	CA	MET	667	49.180	11.960	22.069	1.00	37.60
ATOM	5142	СВ	MET	667	49.150	13.423	21.641	1.00	41.95
ATOM	5143	CG	MET	667	50.487	13.975	21.226	1.00	48.44
ATOM	5144	SD	MET	667	50.384	15.728	20.919	1.00	55.33
ATOM	5145	CE	MET	667	50.711	15.745	19.183	1.00	49.29
ATOM	5146	c	MET	667	48.294	11.802	23.289	1.00	
ATOM	5147	0	MET	667	47.066	11.699	23.283	1.00	38.98
ATOM	5148	N	ALA	668	48.933	11.824			39.18
			AUA	000	10.733	11.024	24.456	1.00	38.72

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MOTA 5150 CA ALA 668 48.231 11.728 1.00 25.727 37.82 MOTA 5151 CB ALA 668 49.224 11.527 26.857 1.00 38.49 MOTA 5152 С ALA 668 47.497 13.051 25.891 1.00 38.16 MOTA 5153 0 ALA 47.937 668 14.072 25.363 1.00 37.21 MOTA 5154 N PRO 669 46.383 13.062 26,644 1.00 39.78 **ATOM** 5155 CD **PRO** 669 45.785 11.931 27.367 1.00 40.08 **ATOM** 5156 CA **PRO** 669 45.598 14.281 26.858 1.00 40.68 MOTA 5157 CB PRO 669 44.474 13.806 27.782 1.00 42.15 MOTA 5158 CG PRO 669 44.346 12.352 27.446 1.00 42.56 **ATOM** 5159 С PRO 669 46.398 15.432 27.484 1.00 42.69 MOTA 5160 0 PRO 669 46.320 16.566 27.019 1.00 42.14 **ATOM** 5161 N GLU 670 47.168 15.153 28.532 1.00 43.21 MOTA 5163 CA GLU 670 47.956 16.211 29.160 1.00 44.62 MOTA 5164 CB 48.651 15.719 30.429 1.00 GLU 670 44.95 MOTA 5165 CG GLU 670 49.824 14.782 30.197 1.00 45.54 MOTA GLU 5166 CD 49.422 670 13.332 30.079 1.00 42.72 MOTA 5167 OE1 GLU 670 50.332 12.481 30.066 1.00 41.43 MOTA 48.212 5168 OE2 GLU 670 30.015 13.036 1.00 44.44 MOTA 5169 C 670 GLU 48.993 16.772 28.195 1.00 44.88 MOTA 5170 0 GLU 670 49.248 17.968 28.194 1.00 45.08 MOTA 5171 N ALA 671 49.565 15.908 27.358 1.00 44.75 MOTA 5173 CA ALA 671 50.573 16.323 26.392 1.00 45.92 MOTA 5174 CB ALA 671 51.256 15.095 25.766 1.00 44.10 MOTA 5175 C ALA 671 49.944 17.193 25.314 1.00 47.96 MOTA 5176 18.192 0 ALA 671 50.526 24.894 1.00 49.16 MOTA 5177 N LEU 672 48.729 16.836 24.917 1.00 49.84 **ATOM** 5179 CA LEU 672 47.989 17.554 23.881 1.00 50.74 **ATOM** 5180 CB LEU 672 46.926 16.619 23.289 1.00 53.20 MOTA 5181 CG LEU 672 46.184 16.989 22.004 1.00 55.26 **ATOM** 5182 CD1 LEU 672 47.153 17.155 20.856 1.00 57.12 MOTA 5183 CD2 LEU 672 45.203 15.895 21.680 1.00 52.86 MOTA 5184 С LEU 672 47.327 18.826 24.408 1.00 50.79 MOTA 5185 0 LEU 672 47.302 19.855 23.736 1.00 50.95 **ATOM** 5186 N PHE 673 46.792 18.751 25.618 1.00 52.07 MOTA 5188 CA PHE 673 46.111 19.884 26.226 1.00 54.39 MOTA 5189 44.892 CB PHE 673 19.396 27.019 1.00 51.21 **ATOM** 5190 CGPHE 673 43.871 18.656 26.186 1.00 48.49 MOTA 5191 CD1 PHE 673 43.304 17.473 26.646 1.00 47.79 MOTA 5192 CD2 PHE 673 43.470 19.149 24.949 1.00 49.04 MOTA 5193 CE1 PHE 673 42.349 16.789 25.888 47.90 1.00 MOTA 5194 CE2 PHE 673 42.511 18.473 24.182 1.00 49.71 MOTA 5195 CZPHE 673 41.952 17.288 24.655 1.00 46.86 MOTA 5196 PHE 673 47.007 C 20.741 27.123 1.00 58.25 ATOM 5197 0 PHE 673 47.000 21.971 27.034 1.00 60.52 ATOM 5198 ASP N 674 47.784 20.094 27.983 1.00 59.63 MOTA 5200 CA ASP 674 48.652 20.815 28.905 1.00 62.11 MOTA 5201 CB ASP 674 48.568 20.196 30.307 1.00 63.81 MOTA 674 47.143 5202 CG ASP 20.015 30.791 1.00 66.46 MOTA 5203 OD1 **ASP** 674 46.815 18.901 31.247 1.00 66.70 MOTA 5204 OD2 ASP 46.354 674 20.981 30.722 1.00 68.77 ATOM 5205 С ASP 674 50.119 20.852 28.482 1.00 63.36 ATOM 5206 0 ASP 50.979 674 21.175 29.310 1.00 64.11 ATOM 5207 N ARG 675 50.410 20.486 27.228 1.00 62.94 MOTA 5209 ARG CA 675 51.789 20.456 26.706

1.00

60.75

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ATOM	5210	CB	ARG	675	52.277	21.874	26.360	1.00	60.56
ATOM	5211	CG	ARG	675	51.474	22.560	25.261	1.00	63.67
MOTA	5212	CD	ARG	675	51.986	23.970	24.964	1.00	66.99
ATOM	5213	NE	ARG	675	53.308	23.980	24.337	1.00	69.34
MOTA	5215	CZ	ARG	675	54.063	25.068	24.173	1.00	68.48
ATOM	5216	NH1	ARG	675	53.637	26.254	24.590	1.00	65.81
ATOM	5219	NH2	ARG	675	55.254	24.965	23.593	1.00	68.76
ATOM	5222	С	ARG	675	52.750	19.793	27.700	1.00	58.06
ATOM	5223	О	ARG	675	53.933	20.130	27.766	1.00	59.30
ATOM	5224	N	ILE	676	52.221	18.859	28.483	1.00	55.62
MOTA	5226	CA	ILE	676	52.992	18.141	29.489	1.00	54.09
ATOM	5227	СВ	ILE	676	52.154	17.921	30.765	1.00	52.69
ATOM	5228	CG2	ILE	676	52.749	16.811	31.629	1.00	49.38
ATOM	5229	CG1	ILE	÷676	52.049	19.230	31.540	1.00	53.15
MOTA	5230	CD1	ILE	676	51.306	19.103	32.845	1.00	57.79
ATOM	5231	C	ILE	676	53.468	16.796	28.953	1.00	53.83
ATOM	5232	0	ILE	676	52.668	15.891	28.730	1.00	54.87
ATOM	5233	N	TYR	677	54.773	16.671	28.745	1.00	51.76
ATOM	5235	CA	TYR	677	55.343	15.436	28.236	1.00	49.42
ATOM	5236	CB	TYR	677	56.232	15.722	27.031	1.00	51.33
MOTA MOTA	5237 5238	CG	TYR	677	55.466	16.181	25.809	1.00	56.22
ATOM	5238	CD1 CE1	TYR	677	55.158	17.529	25.619	1.00	56.12
ATOM	5240	CD2	TYR TYR	677	54.491	17.960	24.479	1.00	56.18
ATOM	5241	CE2	TYR	677 677	55.078	15.269	24.823	1.00	58.13
ATOM	5242	CEZ	TYR	677	54.411 54.125	15.689	23.679	1.00	57.65
ATOM	5243	OH	TYR	677	53.504	17.035	23.512	1.00	58.23
ATOM	5245	c	TYR	677	56.136	17.457	22.360	1.00	61.71
ATOM	5246	0	TYR	677	56.983	14.730 15.335	29.316 29.970	1.00	46.46
ATOM	5247	N	THR	678	55.818	13.355	29.570	1.00 1.00	48.65
ATOM	5249	CA	THR	678	56.498	12.664	30.535	1.00	41.73 39.83
ATOM	5250	СВ	THR	678	55.680	12.593	31.861	1.00	41.78
MOTA	5251	OG1	THR	678	54.462	11.867	31.642	1.00	45.77
ATOM	5253	CG2	THR	678	55.342	13.988	32.383	1.00	41.84
ATOM	5254	С	THR	678	56.661	11.242	30.011	1.00	37.46
ATOM	5255	0	THR	678	56.258	10.917	28.897	1.00	37.51
MOTA	5256	N	HIS	679	57.264	10.388	30.825	1.00	36.36
MOTA	5258	CA	HIS	679	57.423	9.003	30.457	1.00	35.91
MOTA	5259	СВ	HIS	679	58.348	8.294	31.439	1.00	35.05
ATOM	5260	CG	HIS	679	59.761	8.798	31.404	1.00	37.68
ATOM	5261	CD2	HIS	679	60.453	9.569	32.278	1.00	37.89
ATOM	5262	ND1	HIS	679	60.632	8.507	30.380	1.00	37.49
ATOM	5264	CE1	HIS	679	61.803	9.071	30.621	1.00	39.58
ATOM	5265	NE2	HIS	679	61.721	9.722	31.766	1.00	39.81
ATOM	5267	С	HIS	679	56.032	8.376	30.441	1.00	36.76
ATOM	5268	0	HIS	679	55.771	7.458	29.660	1.00	37.16
ATOM	5269	N	GLN	680	55.126	8.908	31.264	1.00	36.27
ATOM	5271	CA	GLN	680	53.754	8.407	31.332	1.00	37.71
MOTA	5272	CB	GLN	680	53.069	8.815	32.640	1.00	40.95
MOTA	5273	CG	GLN	680	53.645	8.128	33.884	1.00	45.23
ATOM	5274	CD	GLN	680	53.676	6.595	33.780	1.00	44.44
ATOM	5275	OE1	GLN	680	52.669	5.925	33.996	1.00	42.76
ATOM	5276	NE2	GLN	680	54.846	6.043	33.464	1.00	40.57
MOTA	5279	С	GLN	680	52.927	8.842	30.121	1.00	37.54

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5280 MOTA 0 GLN 680 51.950 8.185 29.765 1.00 37.93 N MOTA 5281 SER 681 53.282 9.961 29.504 1.00 36.38 **ATOM** 5283 CA SER 681 52.563 10.367 28.306 1.00 38.05 **ATOM** 5284 CB SER 681 52.857 11.819 27.940 1.00 41.41 ATOM 5285 OG SER 681 54.239 12.069 27.938 1.00 42.92 MOTA 5287 C SER 681 52.991 9.421 27.178 1.00 37.92 MOTA 5288 SER O 681 52.205 9.148 26.263 1.00 37.21 MOTA ASP 5289 N 682 54.237 8.932 27.248 1.00 34.77 ATOM 5291 CA ASP 682 54.750 7.972 26.267 1.00 31.99 MOTA 5292 CB ASP 682 56.243 7.683 26.481 1.00 31.08 ATOM 5293 CG ASP 682 57.165 8.638 25.721 1.00 33.63 MOTA 5294 OD1 ASP 682 58.386 8.503 25.920 1.00 32.35 MOTA 5295 OD2 ASP 682 56.707 9.500 24.930 1.00 29.46 MOTA 5296 C 682 ... ASP 53.969 6.672 26.457 1.00 31.54 MOTA 5297 0 ASP 682 53.675 5.971 25.493 1.00 29.94 MOTA 5298 N VAL 683 53.677 6.334 27.712 1.00 30.48 MOTA 5300 CA VAL 683 52.913 5.126 28.023 1.00 32.94 MOTA 5301 CB VAL 683 52.731 4.939 29.572 1.00 33.94 ATOM 5302 CG1 VAL 683 51.635 3.905 29.872 1.00 32.71 MOTA 5303 CG2 VAL 683 54.042 4.474 30.209 1.00 27.41 MOTA 5304 С VAL 683 51.545 5.164 27.299 1.00 32.27 MOTA 5305 VAL O 683 51.106 4.158 26.733 1.00 30.54 MOTA 5306 TRP N 684 50.902 6.332 27.282 1.00 32.57 MOTA 5308 CA TRP 684 49.616 6.477 26.600 1.00 32.76 MOTA 5309 CB TRP 684 49.060 7.895 26.765 1.00 33.67 MOTA 5310 CG TRP 684 47.855 8.210 25.891 1.00 38.22 CD2 MOTA 5311 TRP 684 46.503 8.435 26.328 1.00 39.96 ATOM 5312 CE₂ TRP 684 45.734 8.735 25.177 1.00 39.59 ATOM 5313 CE3 TRP 684 45.869 8.416 27.578 1.00 39.26 MOTA 5314 CD1 TRP 684 47.842 **B.373** 24.528 1.00 39.02 MOTA 5315 NE1 TRP 684 46.576 8.687 24.096 1.00 38.42 MOTA 5317 CZ2 TRP 684 44.362 9.011 25.240 1.00 36.62 MOTA 5318 CZ3 TRP 684 44.502 8.691 27.641 1.00 40.70 MOTA 5319 CH2 TRP 43.766 684 8.982 26.475 1.00 40.57 MOTA 5320 TRP C 684 49.819 6.158 25.125 1.00 31.98 MOTA 5321 0 TRP 684 49.066 5.367 24.557 1.00 32.43 MOTA 5322 N SER **6B5** 50.859 6.748 24.529 1.00 29.63 MOTA 5324 CA SER 685 51.195 6.531 23.119 1.00 28.62 MOTA 5325 CB SER 685 52.457 7.296 22.751 1.00 24.72 MOTA 5326 OG SER 685 52.323 8.664 23.072 1.00 30.04 MOTA 5328 С SER 685 51.414 5.055 22.825 1.00 27.91 **ATOM** 5329 0 SER 685 51.022 4.555 21.767 1.00 28.60 ATOM 5330 N PHE 686 52.063 4.372 23.763 1.00 27.96 MOTA 5332 CA PHE 686 52.333 2.947 23.662 1.00 27.03 **ATOM** 5333 CB PHE 686 53.163 2.499 24.868 1.00 25.79 **ATOM** 5334 CG PHE 686 53.440 1.029 24.890 1.00 26.25 MOTA 5335 CD1 PHE 686 54.252 0.451 23.923 1.00 27.32 MOTA 5336 CD2 PHE 686 52.839 0.208 25.841 1.00 26.22 MOTA 5337 CE1 PHE 686 54.464 -0.930 23.900 1.00 25.87 ATOM 5338 CE2 PHE 686 53.046 -1.170 25.828 1.00 24.37 MOTA 5339 PHE CZ 686 53.856 -1.740 24.854 1.00 26.42 MOTA 5340 С PHE 686 51.003 2.160 23.596 1.00 28.82 MOTA 5341 0 PHE 686 50.912 1.129 22.914 1.00 26.74 MOTA 5342 N GLY 687 49.991 2.636 24.324 1.00 29.52

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ATOM	5344	CA	GLY	687	48.688	1.982	24.302	1.00	31.57
MOTA	5345	C	GLY	687	48.095	2.036	22.896	1.00	30.73
MOTA	5346	0	GLY	687	47.490	1.069	22.414	1.00	29.83
MOTA	5347	N	VAL	688	48.269	3.179	22.238	1.00	29.06
MOTA	5349	CA	VAL	688	47.777	3.350	20.879	1.00	28.93
MOTA	5350	CB	VAL	688	47.800	4.831	20.424	1.00	27.24
MOTA	5351	CG1	VAL	688	47.211	4.963	19.020	1.00	28.29
ATOM	5352	CG2	VAL	688	46.990	5.691	21.404	1.00	26.96
MOTA	5353	C	VAL	688	48.612	2.475	19.951	1.00	28.49
ATOM	5354	0	VAL	688	48.080	1.866	19.024	1.00	28.84
ATOM	5355	N	LEU	689	49.905	2.350	20.252	1.00	27.99
ATOM	5357	CA	LEU	689	50.804	1.512	19.461	1.00	26.14
MOTA	5358	CB	LEU	689	52.268	1.688	19.911	1.00	27.31
MOTA	5359	CG	LEU	689	53.368	1.014	19.065	1.00	26.60
MOTA	5360	CD1	LEU	689	54.688	1.767	19.175	1.00	28.19
MOTA	5361	CD2	LEU	689	53.567	-0.401	19.475	1.00	25.55
MOTA	5362	C	LEU	689	50.362	0.053	19.605	1.00	26.48
ATOM	5363	0	LEU	689	50.377	-0.686	18.626	1.00	27.06
ATOM	5364	N	LEU	690	49.953	-0.344	20.816	1.00	28.55
ATOM	5366	CA	LEU	690	49.465	-1.708	21.085	1.00	29.16
ATOM	5367	CB	LEU	690	49.070	-1.888	22.560	1.00	31.40
ATOM	5368	CG	LEU	690	50.114	-2.085	23.667	1.00	31.49
ATOM	5369	CD1	LEU	690	49.427	-2.028	25.026	1.00	34.09
ATOM	5370	CD2	LEU	690	50.821	-3.410	23.491	1.00	30.84
MOTA	5371	C	LEU	690	48.240	-1.958	20.220	1.00	26.51
ATOM	5372	0	LEU	690	48.088	-3.023	19.631	1.00	25.15
ATOM	5373	N	TRP	691	47.376	-0.954	20.139	1.00	28.51
ATOM	5375	CA	TRP	691	46.169	-1.049	19.319	1.00	29.56
ATOM	5376	СВ	TRP	691	45.332	0.227	19.465	1.00	28.91
ATOM	5377	CG	TRP	691	43.992	0.169	18.759	1.00	30.95
ATOM	5378	CD2	TRP	691	43.718	0.556	17.406	1.00	29.87
ATOM	5379	CE2	TRP	691	42.337	0.367	17.189	1.00	31.97
MOTA	5380	CE3	TRP	691	44.505	1.049	16.358	1.00	27.72
ATOM	5381	CD1	TRP	691	42.796	-0.231	19.292	1.00	30.68
ATOM	5382	NE1	TRP	691	41.797	-0.111	18.355	1.00	33.68
ATOM	5384	CZ2	TRP	691	41.729	0.652	15.967	1.00	29.42
MOTA MOTA	5385	CZ3	TRP	691	43.906	1.327	15.154	1.00	27.13
ATOM	5386 5387	CH2 C	TRP TRP	691 691	42.523	1.129	14.965	1.00	29.18
ATOM	5388	0	TRP	691	46.564	-1.289	17.856	1.00	28.78
ATOM	5389	N	GLU	692	45.996 47.564	-2.156	17.194 17.380	1.00 1.00	27.64
ATOM	5391	CA	GLU	692	48.078	-0.543			29.83
ATOM	5392	CB	GLU	692	49.267	-0.669 0.262	16.018 15.790	1.00 1.00	28.08
ATOM	5393	CG	GLU	692	48.945	1.735	15.680	1.00	26.40 26.45
ATOM	5394	CD	GLU	692	50.183	2.561	15.369	1.00	29.47
ATOM	5395	OE1	GLU	692	50.183	2.886	16.320	1.00	29.47
ATOM	5396	OE2	GLU	692	50.413	2.875	14.182	1.00	
ATOM	5397	C	GLU	692	48.563	-2.082	15.761	1.00	29.44 30.07
ATOM	5398	0	GLU	692	48.385	-2.612	14.665	1.00	30.07
ATOM	5399	N	ILE	693	49.244	-2.663	16.746	1.00	29.87
ATOM	5401	CA	ILE	693	49.754	-4.024	16.608	1.00	29.51
ATOM	5402	СВ	ILE	693	50.632	-4.443	17.828	1.00	28.18
ATOM	5403	CG2	ILE	693	51.037	-5.907	17.706	1.00	27.45
ATOM	5404	CG1	ILE	693	51.907	-3.594	17.890	1.00	26.99

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5405 CD1 MOTA ILE 693 52.663 -3.747 19.194 1.00 25.37 MOTA 5406 C ILE 693 48.603 -5.023 16.452 1.00 29.21 MOTA 5407 0 ILE 693 48.568 -5.807 15.512 1.00 27.89 MOTA 5408 N PHE 694 -4.942 17.336 1.00 47.623 31.33 MOTA 5410 CA PHE 694 46.523 -5.888 17.279 1.00 34.41 MOTA 5411 CB PHE 694 45.958 -6.114 18.687 1.00 35.37 MOTA 5412 CG PHE 694 46.978 -6.717 19.621 1.00 35.60 MOTA 5413 CD1 PHE 694 47.606 -5.942 20.586 1.00 37.23 MOTA 5414 CD2 PHE 694 47.424 -8.024 19.426 1.00 35.59 MOTA 5415 CE1 PHE 694 48.669 -6.460 21.333 1.00 36.39 MOTA 5416 CE2 PHE 694 48.484 -8.546 20.170 1.00 35.34 MOTA 5417 CZPHE 694 49.110 -7.762 1.00 21.118 35.71 MOTA 5418 C PHE 694 45.481 -5.715 16.176 1.00 34.41 **ATOM** 5419 О PHE 694 44.623 -6.579 15.982 1.00 34.48 MOTA 5420 N THR 695 45.617 15.404 -4.637 1.00 33.03 MOTA 5422 CA THR 695 44.742 -4.379 14.263 1.00 31.81 MOTA 5423 CB THR 695 44.113 -2.957 14.278 1.00 29.75 MOTA 5424 OG1 695 THR 45.142 -1.961 14.218 1.00 30.72 MOTA 5426 CG2 THR 695 43.254 -2.759 15.524 1.00 29.40 MOTA 5427 C THR 695 45.596 -4.533 13.011 1.00 31.44 **ATOM** 5428 O THR 695 45.153 -4.241 11.906 1.00 33.00 **ATOM** 5429 N LEU 696 46.832 -4.987 13.209 1.00 31.24 ATOM 5431 CA LEU 696 47.799 -5.199 12.134 1.00 31.36 MOTA 5432 CB LEU 696 47.421 -6.418 11.291 1.00 33.53 MOTA 5433 CG LEU 696 47.270 -7.741 12.042 1.00 33.00 MOTA 5434 LEU CD1 696 47.010 ~8.838 11.052 1.00 35.50 MOTA 5435 CD2 LEU 696 36.09 48.515 -8.061 12.830 1.00 MOTA 5436 C LEU 696 48.066 -3.976 11.249 1.00 30.84 MOTA 5437 0 LEU 696 48.135 -4.067 10.024 1.00 28.23 ATOM 5438 N GLY 697 48.302 -2.839 11.890 1.00 31.54 MOTA 5440 CA GLY 697 48.591 -1.632 11.141 1.00 33.87 MOTA 5441 С GLY 697 47.375 -0.765 10.924 1.00 32.77 MOTA 5442 0 GLY 697 47.322 0.042 9.994 1.00 33.90 MOTA 5443 N GLY 698 46.392 -0.921 11.797 1.00 33.29 MOTA 5445 CA GLY 698 45.187 -0.122 11.681 1.00 32.66 MOTA 5446 GLY C 698 45.408 1.368 11.877 1.00 30.57 MOTA 5447 0 GLY 69B 46.336 1.803 27.36 12.553 1.00 MOTA 5448 SER 699 N 44.517 2.148 11.285 1.00 30.92 MOTA 5450 CA SER 699 44.552 3.595 11.376 1.00 32.19 MOTA 5451 CB SER 699 44.062 4.202 10.058 1.00 34.24 MOTA 5452 OG SER 699 44.019 5.616 10.123 1.00 38.67 MOTA 5454 C SER 699 43.644 4.014 12.538 1.00 31.81 MOTA 5455 0 SER 699 42.431 3.759 12.525 1.00 31.39 ATOM 5456 N PRO 700 44.228 4.597 13.594 1.00 31.82 ATOM 5457 CD PRO 700 45.645 4.842 13.919 1.00 28.82 MOTA 5458 CA PRO 700 43.353 4.992 14.697 1.00 31.31 MOTA 5459 CB PRO 700 44.345 5.341 15.809 1.00 31.31 MOTA 5460 CG PRO 700 45.552 5.800 15.061 1.00 30.41 MOTA 5461 С PRO 700 42.484 6.170 14.295 1.00 31.19 MOTA 5462 0 PRO 700 42.899 7.021 13.510 1.00 29.93 **ATOM** 5463 N TYR 701 41.235 6.144 14.736 1.00 32.69 MOTA 5465 CA TYR 701 40.291 7.223 14.445 1.00 32.54 ATOM 5466 CB TYR 701 40.650 8.416 15.323 1.00 34.47 MOTA 5467 CG TYR 701 40.512 8.141 16.794 1.00 39.16

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ATOM	5468	CD1	TYR	701	41.542	8.433	17.683	1.00	44.31
MOTA	5469	CE1	TYR	701	41.372	8.241	19.060	1.00	46.65
ATOM	5470	CD2	TYR	701	39.321	7.642	17.307	1.00	41.21
MOTA	5471	CE2	TYR	701	39.147	7.447	18.657	1.00	45.05
MOTA	5472	CZ	TYR	701	40.164	7.750	19.535	1.00	47.24
MOTA	5473	ОН	TYR	701	39.949	7.590	20.886	1.00	52.18
MOTA	5475	C	TYR	701	40.215	7.655	12.972	1.00	30.56
MOTA	5476	О	TYR	701	40.379	8.836	12.647	1.00	29.73
ATOM	5477	N	PRO	702	39.928	6.712	12.058	1.00	30.38
ATOM	5478	CD	PRO	702	39.659	5.278	12.261	1.00	30.22
ATOM	5479	CA	PRO	702	39.847	7.071	10.642	1.00	28.87
ATOM	5480	CB	PRO	702	39.693	5.722	9.948	1.00	29.63
MOTA	5481	CG	PRO	702	39.007	4.889	10.959	1.00	30.99
MOTA	5482	С	· PRO	702	38.722	8.048	10.283	1.00	30.88
ATOM	5483	0	PRO	702	37.557	7.843	10.636	1.00	33.98
MOTA	5484	N	GLY	703	39.100	9.116	9.584	1.00	29.03
ATOM	5486	CA	GLY	703	38.154	10.134	9.169	1.00	28.98
ATOM	5487	C	GLY	703	37.893	11.169	10.244	1.00	29.69
MOTA	5488	0	GLY	703	37.074	12.068	10.048	1.00	31.71
MOTA	5489	N	VAL	704	38.579	11.040	11.378	1.00	30.74
ATOM	5491	CA	VAL	704	38.416	11.951	12.509	1.00	32.06
ATOM	5492	CB	VAL	704	38.582	11.208	13.860	1.00	31.70
ATOM	5493	CG1	VAL	704	30.522	12.197	15.044	1.00	30.29
ATOM	5494	CG2	VAL	704	37.506	10.144	14.005	1.00	31.56
ATOM	5495	C	VAL	704	39.430	13.087	12.449	1.00	33.72
MOTA	5496	0	VAL	704	40.634	12.867	12.548	1.00	35.31
MOTA	5497	N	PRO	705	38.957	14.309	12.200	1.00	34.23
MOTA	5498	CD	PRO	705	37.594	14.692	11.787	1.00	33.20
ATOM ATOM	5499	CA	PRO	705	39.875	15.443	12.135	1.00	33.73
ATOM	5500	CB	PRO	705	39.053	16.495	11.394	1.00	34.93
ATOM	5501 5502	CG C	PRO	705	37.647	16.187	11.831	1.00	36.93
ATOM	5502 5503	0	PRO PRO	705 705	40.280	15.879	13.543	1.00	33.25
ATOM	5504	N	VAL	705 706	39.651	15.490	14.532	1.00	31.71
ATOM	5504	CA	VAL	706	41.322	16.697	13.623	1.00	34.46
ATOM	5507	СВ	VAL	706	41.852 42.923	17.176 18.261	14.900	1.00	36.99
ATOM	5508	CG1	VAL	706	43.577	18.618	14.687 16.017	1.00	39.01
ATOM	5509	CG2	VAL	706	43.961	17.786	13.673		40.33
ATOM	5510	C	VAL	706	40.826	17.716	15.895	1.00	38.61
ATOM	5511	ō	VAL	706	40.823	17.319	17.065	1.00	35.65 33.55
ATOM	5512	N	GLU	707	39.955	18.605	15.426	1.00	36.74
ATOM	5514	CA	GLU	707	38.941	19.220	16.278	1.00	37.20
MOTA	5515	СВ	GLU	707	38.129	20.242	15.482	1.00	38.98
ATOM	5516	C	GLU	707	38.014	18.188	16.900	1.00	38.46
ATOM	5517	0	GLU	707	37.634	18.295	18.074	1.00	39.04
ATOM	5518	N	GLU	708	37.681	17.170	16.115	1.00	37.81
ATOM	5520	CA	GLU	708	36.802	16.105	16.571	1.00	37.70
ATOM	5521	CB	GLU	708	36.316	15.289	15.378	1.00	40.73
ATOM	5522	CG	GLU	708	35.459	16.091	14.413	1.00	40.73
ATOM	5523	CD	GLU	708	34.235	16.677	15.084	1.00	
ATOM	5524	OE1	GLU	708	33.629	16.007	15.064	1.00	51.52
ATOM	5525	OE2	GLU	708	33.882	17.824	14.732	1.00	50.14
ATOM	5526	C	GLU	708	37.506	15.223	17.588	1.00	59.46
ATOM	5527	0	GLU	708	36.897	14.782	18.567		36.53
	JJ21	_	Guo	, 00	30.031	13.702	10.30/	1.00	36.BO

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38.799 LEU 709 14.993 17.376 1.00 35.69 MOTA 5528 N LEU 709 14.179 18.301 1.00 35.48 MOTA 5530 CA 39.584 1.00 MOTA 5531 CB LEU 709 41.039 14.044 17.830 34.84 709 18.802 1.00 32.41 MOTA 5532 CG LEU 41.921 13.250 LEU 709 41.608 11.787 18.674 1.00 30.10 MOTA 5533 CD1 MOTA 5534 CD2 LEU 709 43.378 13.514 18.560 1.00 29.93 709 MOTA 5535 С LEU 39.568 14.842 19.673 1.00 35.58 MOTA 5536 0 LEU 709 39.377 14.177 20.694 1.00 35.43 MOTA 5537 N PHE 710 39.792 16.150 19.686 1.00 36.79 MOTA 5539 CA PHE 710 39.800 16.918 20.927 1.00 40.58 MOTA 5540 CB PHE 710 39.944 18.413 20.637 1.00 42.55 MOTA 5541 CG PHE 710 41.308 18.808 20.162 1.00 46.38 **ATOM** 5542 CD1 PHE 710 42.392 17.942 20.313 1.00 47.29 5543 - CD2 47.93 MOTA PHE 710 41.515 20.050 19.5B0 1.00 MOTA 5544 CE1 PHE 710 43.659 18.312 19.892 1.00 51.21 1.00 MOTA 5545 CE₂ PHE 710 42.781 20.435 19.155 50.89 MOTA 710 5546 CZ PHE 43.859 19.562 19.312 1.00 53.31 MOTA 5547 C PHE 710 38.517 16.676 21.694 1.00 40.14 MOTA 5548 0 PHE 710 38.543 16.446 22.898 1.00 39.86 MOTA 5549 N LYS 711 37.399 16.705 20.977 1.00 41.02 ATOM 5551 CA LYS 711 36.101 16.479 21.584 1.00 38.66 MOTA 5552 CB LYS 711 34.985 16.803 20.580 1.00 40.75 MOTA 5553 CG LYS 711 16.727 1.00 33.601 21.181 46.99 MOTA 5554 CD LYS 711 32.522 17.174 20.218 1.00 50.71 MOTA 5555 CE LYS 711 31.163 16.733 20.739 1.00 52.53 MOTA 5556 NZ LYS 711 30.041 17.194 19.884 1.00 57.76 MOTA 5560 С LYS 711 35.990 15.046 22.120 1.00 38.06 5561 MOTA 0 LYS 711 35.535 14.831 23.250 1.00 36.29 MOTA 5562 N LEU 712 14.066 21.330 1.00 36.431 38.10 MOTA 5564 LEU CA 712 36.392 12.662 21.764 1.00 38.69 11.714 MOTA 5565 CB LEU 712 20.672 1.00 36.914 37.19 MOTA 712 5566 CG LEU 36.070 11.436 19.424 1.00 34.73 MOTA 5567 LEU CD1 712 36.814 10.453 18.524 1.00 35.54 MOTA 5568 CD2 LEU 19.818 30.90 712 34.709 10.872 1.00 MOTA 5569 C LEU 712 37.230 12.472 23.021 1.00 39.62 MOTA 5570 0 **TEN** 712 36.843 11.745 23.940 1.00 39.44 ATOM 5571 N LEU 713 38.398 13.101 23.044 1.00 40.10 MOTA 5573 LEU CA 713 39.279 12.999 24.199 1.00 42.81 MOTA 5574 CB LEU 713 40.606 13.716 23.924 1.00 41.70 MOTA 5575 CG LEU 22.868 41.86 713 41.495 13.040 1.00 ATOM 5576 CD1 LEU 42.742 22.607 713 13.862 1.00 37.19 MOTA 5577 CD2 LEU 41.873 23.340 713 11.647 1.00 41.17 MOTA 5578 LEU С 713 38.577 13.566 25.437 1.00 43.18 MOTA 5579 0 LEU 713 38.479 12.889 26.457 1.00 44.79 ATOM 5580 N LYS 714 38.004 14.760 25.312 1.00 42.75 MOTA 5582 CA LYS 714 37.301 15.389 26.425 1.00 43.70 MOTA 5583 CB LYS 714 36.842 16.796 26.043 1.00 44.69 MOTA 5584 CG LYS 714 38.001 17.746 25.836 1.00 47.92 MOTA 5585 CDLYS 714 37.543 19.171 25.583 1.00 55.01 MOTA 5586 CE LYS 714 38.733 20.077 25.238 1.00 59.44 **ATOM** 5587 NZ LYS 714 39.773 20.132 26.320 1.00 60.10 MOTA 5591 С LYS 714 36.127 14.557 26.940 1.00 43.94 MOTA 5592 LYS 0 714 35.843 14.551 28.140 1.00 44.20 MOTA

5593

N

GLU

715

35.477

13.819

26.046

1.00

43.29

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MOTA	5595	CA	GLU	715	34.350	12.979	26.435	1.00	42.29
MOTA	5596	CB	GLU	715	33.464	12.682	25.225	1.00	44.91
ATOM	5597	CG	GLU	715	32.913	13.916	24.522	1.00	51.62
MOTA	5598	CD	GLU	715	32.020	13.566	23.332	1.00	55.01
MOTA	5599	OE1	GLU	715	32.343	12.605	22.596	1.00	58.09
MOTA	5600	OE2	GLU	715	30.992	14.251	23.136	1.00	55.83
MOTA	5601	С	GLU	715	34.806	11.665	27.064	1.00	41.07
MOTA	5602	0	GLU	715	33.982	10.825	27.421	1.00	38.01
MOTA	5603	N	GLY	716	36.118	11.476	27.182	1.00	41.11
MOTA	5605	CA	GLY	716	36.642	10.252	27.770	1.00	39.69
MOTA	5606	С	GLY	716	36.510	9.054	26.847	1.00	39.64
ATOM	5607	0	GLY	716	36.562	7.904	27.290	1.00	36.71
MOTA	5608	N	HIS	717	36.359	9.335	25.554	1.00	41.95
ATOM	5610	CA ·	HIS	717	36.215	8.300	24.541	1.00	43.32
ATOM	5611	CB	HIS	717	35.859	8.918	23.183	1.00	43.38
ATOM	5612	CG	HIS	717	35.813	7.926	22.060	1.00	44.79
ATOM	5613	CD2	HIS	717	34.802	7.152	21.596	1.00	44.64
ATOM	5614	NDl	HIS	717	36.912	7.625	21.285	1.00	46.21
ATOM	5616	CE1	HIS	717	36.584	6.708	20.392	1.00	46.21
ATOM	5617	NE2	HIS	717	35.307	6.404	20.561	1.00	45.55
ATOM	5619	С	HIS	717	37.485	7.481	24.403	1.00	43.90
ATOM	5620	0	HIS	717	38.581	8.031	24.327	1.00	45.45
ATOM	5621	N	ARG	718	37.304	6.169	24.289	1.00	43.44
ATOM	5623	CA	ARG	718	38.387	5.207	24.139	1.00	42.68
ATOM	5624	СВ	ARG	718	38.500	4.361	25.412	1.00	41.00
MOTA	5625	CG	ARG	718	38.844	5.165	26.658	1.00	40.09
ATOM	5626	CD	ARG	718	40.214	5.825	26.495	1.00	41.06
ATOM	5627	NE	ARG	718	40.658	6.549	27.685	1.00	39.51
ATOM	5629	CZ	ARG	718	40.521	7.861	27.862	1.00	39.90
MOTA	5630	NH1	ARG	718	39.940	8.608	26.931	1.00	36.48
MOTA	5633	NH2	ARG	718	41.024	8.443	28.946	1.00	42.06
ATOM	5636	C	ARG	718	38.080	4.308	22.927	1.00	43.91
MOTA	5637	0	ARG	718	36.911	4.007	22.650	1.00	44.40
MOTA	5638	N	MET	719	39.113	3.933	22.174	1.00	42.56
ATOM	5640	CA	MET	719	38.928	3.079	21.004	1.00	42.82
MOTA	5641	CB	MET	719	40.219	2.964	20.181	1.00	42.59
MOTA	5642	CG	MET	719	40.595	4.221	19.413	1.00	41.15
MOTA	5643	SD	MET	719	42.093	4.079	18.400	1.00	44.11
ATOM	5644	CE	MBT	719	43.323	3.949	19.613	1.00	41.33
ATOM	5645	С	MET	719	38.460	1.694	21.432	1.00	44.74
ATOM	5646	0	MET	719	38.822	1.216	22.516	1.00	41.56
MOTA	5647	N	ASP	720	37.635	1.075	20.582	1.00	45.50
MOTA	5649	CA	ASP	720	37.090	-0.265	20.824	1.00	45.51
ATOM	5650	CB	ASP	720	36.077	-0.660	19.733	1.00	48.60
MOTA	5651	CG	ASP	720	34.811	0.181	19.749	1.00	53.03
MOTA	5652	OD1	ASP	720	34.678	1.082	20.612	1.00	59.61
ATOM	5653	OD2	ASP	720	33.943	-0.067	18.880	1.00	50.58
ATOM	5654	С	ASP	720	38.177	-1.329	20.823	1.00	43.64
ATOM	5655	0	ASP	720	39.235	-1.172	20.199	1.00	43.66
ATOM	5656	N	LYS	721	37.876	-2.436	21.487	1.00	42.90
ATOM	5658	CA	LYS	721	38.784	-3.565	21.555	1.00	42.96
ATOM	5659	CB	LYS	721	38.278	-4.565	22.587	1.00	42.51
ATOM	5660	CG	LYS	721	39.000	-5.888	22.570	1.00	47.68
ATOM	5661	CD	LYS	721	38.445	-6.805	23.628	1.00	51.61
			-10		55.335	5.005	23.020	1.00	21.01

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MOTA 5662 CE LYS 721 38.450 -8.246 23.163 1.00 54.96 **ATOM** 5663 NZ LYS 721 38.165 -9.190 24.282 1.00 59.67 20.182 ATOM 5667 C LYS 721 38.825 -4.215 1.00 43.05 **ATOM** 5668 0 LYS 721 37.779 -4.577 19.625 1.00 46.08 MOTA 5669 N PRO 722 40.025 -4.348 19.601 1.00 43.22 MOTA 5670 CD PRO 722 41.337 -3.872 20.067 1.00 43.52 MOTA 5671 CA PRO 722 40.139 -4.968 18.275 1.00 41.04 MOTA 5672 CB PRO 722 41.631 -4.856 17.965 1.00 40.87 **ATOM** 5673 CG PRO 722 42.074 -3.682 18.764 1.00 42.22 MOTA 5674 C PRO 722 39.726 -6.427 18.346 1.00 39.64 **ATOM** 5675 0 PRO 722 39.730 -7.023 19.425 1.00 37.12 MOTA 5676 SER 723 N 39.311 -6.98217.212 1.00 40.36 MOTA 5678 CA SER 723 38.947 -8.389 17.158 1.00 41.41 MOTA 5679 CB SER 723 -8.707 38.205 15.865 1.00 38.26 ATOM 5680 OG SER 723 39.049 -8.520 14.749 1.00 43.87 MOTA 5682 C SER 723 40.294 -9.102 17.191 1.00 41.54 **MOTA** 5683 0 SER 723 41.284 -8.575 16.703 1.00 40.90 ATOM 5684 N ASN 724 40.338 -10.300 17.750 1.00 44.89 MOTA 5686 CA ASN 724 41.598 -11.019 17.853 1.00 48.14 MOTA -11.202 16.476 5687 CB ASN 724 42.256 1.00 52.43 MOTA 5688 CG 724 ASN 41.682 -12.374 15.715 1.00 57.29 MOTA 5689 OD1 724 ASN 41.637 -13.492 16.225 1.00 61.96 MOTA 5690 ND2 724 ASN 41.218 -12.125 14.500 1.00 60.91 MOTA 5693 C ASN 724 42.509 -10.255 18.811 1.00 48.17 MOTA 5694 0 ASN 724 43.648 -9.918 18.495 1.00 49.88 MOTA 5695 N CYS 725 41.960 -9.935 19.973 1.00 47.12 MOTA 5697 725 46.17 CA CYS 42.686 -9.238 21.010 1.00 ATOM 5698 CB CYS 725 42.569 -7.717 20.862 1.00 44.83 MOTA 5699 SG CYS 725 43.459 -6.813 22.159 1.00 42.51 MOTA 5700 C **CYS** 725 42.017 -9.697 22.294 1.00 45.78 MOTA 5701 O CYS 725 40.803 -9.642 22.423 1.00 44.83 MOTA 5702 N THR 726 42.810 -10.224 23.212 1.00 45.63 ATOM 5704 CA THR 726 42.289 -10.711 24.482 1.00 45.47 MOTA 5705 CB THR 726 43.351 -11.545 25.217 1.00 45.93 MOTA 5706 OG1 726 THR 44.307 -10.651 25.786 1.00 45.04 ATOM 5708 CG2 THR 726 44.061 -12.495 24.233 1.00 42.99 MOTA 5709 С THR 726 41.858 -9.545 25.359 1.00 45.73 **ATOM** 5710 0 THR 726 42.368 -8.445 25.216 1.00 46.91 MOTA 5711 N ASN 727 40.914 -9.789 26.257 1.00 45.93 MOTA 5713 ASN CA 727 40.448 -8.736 27.141 1.00 47.85 ATOM 5714 CB ASN 727 39.300 -9.237 28.022 1.00 54.88 MOTA 5715 CG ASN 727 39.629 -10.544 28.731 1.00 65.11 **ATOM** 5716 OD1 ASN 727 40.737 -10.734 29.229 1.00 70.58 **MOTA** 5717 ND2 ASN 727 38.681 -11.472 28.735 1.00 69.68 **ATOM** 5720 C ASN 727 41.591 -8.212 27.999 1.00 44.18 **ATOM** 5721 0 ASN 727 41.594 -7.047 28.390 1.00 41.35 **ATOM** 5722 N GLU 728 42.572 -9.073 28.260 1.00 42.82 MOTA 5724 CA GLU 728 43.725 -8.713 29.071 1.00 42.37 MOTA 5725 CB GLU 728 44.573 -9.952 29.379 1.00 43.09 MOTA 5726 CG 728 GLU 45.806 -9.654 30.245 1.00 48.30 **ATOM** 5727 CD **GLU** 728 46.643 -10.889 30.568 1.00 50.11 MOTA 5728 OE1 GLU 728 46.867 -11.732 29.668 1.00 47.98 MOTA 5729 OE2 GLU 728 47.085 -11.010 31.733 1.00 51.69 **MOTA** 5730 C GLU 728 44.551 -7.652 28.356 1.00 39.57

ATOM	5731	0	GĽU	728	44.852	-6.605	28.933	1.00	39.30
ATOM	5732	N	LEU	729	44.872	-7.907	27.089	1.00	37.38
ATOM	5734	CA	LEU	729	45.655	-6.977	26.274	1.00	36.74
ATOM	5735	CB	LEU	729	46.027	-7.623	24.935	1.00	35.39
MOTA	5736	CG	LEU	729	47.137	-8.679	25.001	1.00	35.41
MOTA	5737	CD1	LEU	729	47.107	-9.553	23.766	1.00	35.69
MOTA	5738	CD2	LEU	729	48.505	-8.017	25.174	1.00	37.72
MOTA	5739	С	LEU	729	44.885	-5.679	26.050	1.00	35.52
ATOM	5740	0	LEU	729	45.467	-4.597	25.941	1.00	33.96
ATOM	5741	N	TYR	730	43.565	-5.779	26.000	1.00	32.90
ATOM	5743	CA	TYR	730	42.760	-4.598	25.812	1.00	32.41
ATOM	5744	CB	TYR	730	41.335	-4.981	25.398	1.00	32.16
ATOM	5745	CG	TYR	730	40.445	-3.787	25.172	1.00	34.93
ATOM	5746	CD1.	TYR	730	40.769	-2.827	24.203	1.00	32.49
ATOM	5747	CE1	TYR	730	39.962	-1.716	23.994	1.00	32.80
ATOM	5748	CD2	TYR	730	39.282	-3.605	25.931	1.00	33.45
MOTA	5749	CE2	TYR	730	38.465	-2.496	25.728	1.00	34.81
ATOM	5750	CZ	TYR	730	38.814	-1.557	24.756	1.00	34.06
MOTA	5751 5751	ОН	TYR	730	38.009	-0.465	24.551	1.00	36.66
ATOM	5753 5754	C	TYR	730	42.767	-3.788	27.107	1.00	33.48
ATOM ATOM	5754 5755	0	TYR	730	42.837	-2.558	27.083	1.00	34.94
ATOM	5757	N CA	MET	731	42.698	-4.466	28.248	1.00	35.29
ATOM	5758	CB	MET MET	731 731	42.724	-3.755	29.525	1.00	38.38
ATOM	5759	CG	MET	731	42.465	-4.709	30.690	1.00	42.01
ATOM	5760	SD	MET	731	41.048 39.785	-5.264 -3.965	30.702	1.00	53.67
ATOM	5761	CE	MET	731	39.828	-3.688	30.830	1.00	62.97
ATOM	5762	C	MET	731	44.073	-3.049	32.641	1.00	61.83
ATOM	5763	ō	MET	731	44.160	-1.958	29.670 30.232	1.00	34.52
ATOM	5764	N	MET	732	45.118	-3.669	29.134	1.00	33.23 33.93
ATOM	5766	CA	MET	732	46.445	-3.065	29.168	1.00	36.26
ATOM	5767	СВ	MET	732	47.506	-3.995	28.565	1.00	35.56
MOTA	5768	CG	MET	732	48.935	-3.418	28.643	1.00	35.26
MOTA	5769	SD	MET	732	50.186	-4.522	28.001	1.00	30.46
MOTA	5770	CE	MET	732	50.480	-5.562	29.415	1.00	26.88
MOTA	5771	C	MET	732	46.369	-1.750	28.389	1.00	34.75
MOTA	5772	0	MET	732	46.827	-0.722	28.873	1.00	35.49
ATOM	5773	N	MET	733	45.741	-1.774	27.213	1.00	34.63
MOTA	5775	CA	MET	733	45.571	-0.566	26.413	1.00	32.79
MOTA	5776	CB	MET	733	44.787	-0.853	25.130	1.00	33.16
MOTA	5777	CG	MET	733	45.544	-1.601	24.047	1.00	32.32
MOTA	5778	SD	MET	733	44.421	-1.990	22.670	1.00	35.66
ATOM	5779	CE	MET	733	45.155	-3.496	22.068	1.00	29.47
MOTA	5780	С	MET	733	44.789	0.452	27.229	1.00	33.94
ATOM	5781	0	MET	733	45.176	1.619	27.318	1.00	35.72
ATOM	5782	N	ARG	734	43.679	0.018	27.818	1.00	33.73
ATOM	5784	CA	ARG	734	42.854	0.913	28.621	1.00	33.41
ATOM	5785	CB	ARG	734	41.586	0.197	29.095	1.00	33.42
ATOM	5786	CG	ARG	734	40.726	-0.335	27.950	1.00	34.26
ATOM	5787	CD	ARG	734	40.256	0.783	27.043	1.00	37.70
ATOM	5788	NE	ARG	734	39.416	1.745	27.750	1.00	43.98
ATOM	5790	CZ	ARG	734	38.092	1.661	27.844	1.00	46.43
ATOM	5791	NHl	ARG	734	37.439	0.660	27.268	1.00	48.63
ATOM	5794	NH2	ARG	734	37.420	2.571	28.530	1.00	44.65

MOTA 5797 C ARG 734 43.660 1.458 29.793 1.00 32.12 MOTA 5798 ARG 734 2.610 0 43.492 30.180 1.00 35.37 MOTA 5799 N **ASP** 735 44.566 0.646 30.327 1.00 33.75 MOTA CA 5801 ASP 735 45.438 1.076 31.433 1.00 36.72 MOTA 5802 CB **ASP** 735 46.379 -0.055 31.857 1.00 42.71 MOTA 5803 CG ASP 735 45.722 -1.052 32.774 1.00 47.31 MOTA 5804 OD1 ASP 735 46.124 -2.241 32,720 1.00 50.99 **ATOM** 5805 OD2 ASP 735 44.824 -0.646 33.552 1.00 48.45 MOTA 5806 C ASP 735 46.291 34.25 2.251 30.972 1.00 MOTA 5807 ASP 735 0 46.376 3.286 31.648 1.00 34.31 MOTA 5808 N CYS 736 46.927 2.064 29.816 1.00 31.85 **ATOM** 5810 CA CYS 736 47.780 3.077 29.204 1.00 29.93 ATOM 5811 CB CYS 736 48.413 2.545 27.921 1.00 24.97 **ATOM** 5812 SG CYS 736 49.504 1.159 28.180 1.00 31.35 MOTA 5813 С CYS 736 46.994 4.325 28.885 1.00 31.62 **MOTA** 5814 0 CYS 736 47.562 5.416 28.823 1.00 30.73 MOTA 5815 N TRP 737 45.680 4.174 28.711 1.00 35.03 **ATOM** 5817 TRP CA 737 44.812 5.308 28.395 1.00 36.35 **ATOM** 5818 CBTRP 737 43.808 4.927 27.297 1.00 36.43 MOTA 5819 CG TRP 737 44.451 4.487 26.010 1.00 34.34 MOTA 5820 CD2 TRP 737 43.914 3.565 25.052 1.00 34.81 MOTA 5821 CE2 TRP 737 44.852 3.461 23.999 1.00 33.92 MOTA 5822 CE3 TRP 737 42.730 2.816 24.980 1.00 33.06 MOTA 5823 CD1 TRP 737 45.659 4.890 25.514 1.00 35.19 MOTA 5824 NE1 TRP 737 45.907 4.279 24.309 1.00 35.00 MOTA 5826 CZ2 TRP 737 44.644 2.633 22.886 1.00 33.45 MOTA 5827 CZ3 TRP 737 42.527 1.991 23.876 1.00 32.92 MOTA 5828 CH2 TRP 737 43.480 1.909 22.844 1.00 30.45 MOTA 5829 С TRP 737 44.080 5.895 29.609 1.00 37.23 MOTA 5830 0 TRP 737 43.047 6.551 29.474 1.00 37.44 MOTA 5831 N HIS 738 44.624 5.681 30.798 1.00 41.45 MOTA 5833 CA HIS 738 44.006 6.208 32.008 1.00 41.52 MOTA 5834 CB HIS 738 44.675 5.635 33.258 1.00 41.23 MOTA 5835 738 CG HIS 43.925 5.924 34.522 1.00 43.31 MOTA 5836 CD2 HIS 738 43.618 7.096 35.126 1.00 41.58 MOTA 5837 ND1 HIS 738 43.338 4.935 35.279 1.00 44.22 MOTA 5839 CE1 HIS 738 42.693 5.487 36.294 1.00 46.62 MOTA 5840 NE2 HIS 738 42.848 6.798 36.223 1.00 43.99 MOTA 5842 С HIS 738 44.118 7.726 32.015 1.00 41.75 ATOM 5843 0 HIS 738 45.179 8.268 31.731 1.00 40.84 5844 **MOTA** N ALA 739 43.025 8.405 32.352 1.00 42.47 **ATOM** 5846 ALA CA 739 43.004 9.873 32.398 1.00 44.58 MOTA 5847 CB **ALA** 739 41.629 10.361 32.825 1.00 48.19 MOTA 5848 C ALA 739 44.081 10.467 33.317 1.00 45.12 MOTA 5849 0 ALA 739 44.653 11.510 33.020 1.00 45.66 MOTA 740 5850 N VAL 44.262 9.852 34.481 1.00 46.64 MOTA 5852 CA VAL 740 45.278 10.273 35.453 1.00 46.78 MOTA 5853 CB VAL 740 44.867 9.893 36,888 1.00 47.74 MOTA 5854 CG1 VAL 740 45.919 10.372 37.890 1.00 49.35 **ATOM** 5855 CG₂ VAL 740 43.515 10.495 37.211 1.00 47.89 MOTA 5856 C VAL 740 46.601 9.573 35.121 1.00 45.24 MOTA 5857 0 VAL 740 46.754 8.362 35.347 1.00 45.01 MOTA 5858 N **PRO** 741 47.588 10.335 34.637 1.00 43.46 MOTA 5859 CD PRO 741 47.536 11.794 34.437 1.00 43.51

ATOM	5860	CA-	PRO	741	48.905	9.804	34.266	1.00	46.22
MOTA	5861	CB	PRO	741	49.701	11.070	33.942	1.00	45.32
MOTA	5862	CG	PRO	741	48.632	12.010	33.426	1.00	42.81
ATOM	5863	С	PRO	741	49.588	8.936	35.328	1.00	47.45
ATOM	5864	0	PRO	741	50.245	7.950	34.994	1.00	45.12
ATOM	5865	N	SER	742	49.394	9.280	36.601	1.00	48.78
ATOM	5867	CA	SER	742	49.994	8.532	37.703	1.00	48.76
MOTA	5868	CB	SER	742	49.845	9.317	39.012	1.00	51.11
MOTA	5869	OG	SER	742	48.482	9.488	39.373	1.00	53.50
ATOM	5871	С	SER	742	49.376	7.150	37.867	1.00	47.77
ATOM	5872	0	SER	742	49.932	6.283	38.539	1.00	47.31
MOTA	5873	N	GLN	743	48.199	6.962	37.284	1.00	47.57
MOTA	5875	CA	GLN	743	47.511	5.689	37.384	1.00	47.14
MOTA	5876	CB	GLN	743	46.004	5.918	37.531	1.00	50.16
MOTA	5877	CG	GLN	743	45.438	5.447	38.871	1.00	54.69
ATOM	5878	CD	GLN	743	46.239	5.964	40.051	1.00	57.62
ATOM	5879	OE1	GLN	743	46.898	5.196	40.749	1.00	59.09
ATOM	5880	NE2	GLN	743	46.202	7.277	40.268	1.00	59.45
MOTA	5883	С	GLN	743	47.816	4.774	36.212	1.00	44.41
ATOM	5884	O	GLN	743	47.365	3.627	36.182	1.00	44.39
ATOM	5885	N	ARG	744	48.515	5.305	35.212	1.00	42.87
ATOM	5887	CA	ARG	744	48.902	4.506	34.046	1.00	41.45
ATOM	5888	СВ	ARG	744	49.350	5.397	32.883	1.00	37.34
MOTA	5889	CG	ARG	744	48.316	6.380	32.412	1.00	32.30
ATOM	5890	CD	ARG	744	48.854	7.207	31.270	1.00	31.37
MOTA	5891	NE	ARG	744	47.921	8.276	30.946	1.00	36.76
ATOM	5893	CZ	ARG	744	48.271	9.492	30.543	1.00	39.88
ATOM	5894	NH1	ARG	744	49.553	9.813	30.399	1.00	39.94
MOTA	5897	NH2	ARG	744	47.330	10.404	30.322	1.00	39.12
MOTA	5900	С	ARG	744	50.068	3.616	34.471	1.00	41.40
MOTA	5901	0	ARG	744	50.813	3.945	35.405	1.00	42.84
ATOM	5902	N	PRO	745	50.203	2.441	33.849	1.00	40.11
ATOM	5903	CD	PRO	745	49.345	1.739	32.876	1.00	39.91
ATOM	5904	CA	PRO	745	51.332	1.607	34.266	1.00	38.58
ATOM	5905	CB	PRO	745	51. 01 9	0.261	33.605	1.00	37.46
MOTA	5906	CG	PRO	745	50.250	0.645	32.377	1.00	37.41
ATOM	5907	C	PRO	745	52.640	2.202	33.750	1.00	37.73
MOTA	5908	0	PRO	745	52.634	3.027	32.835	1.00	37.71
MOTA	5909	N	THR	746	53.753	1.843	34.373	1.00	35.90
MOTA	5911	CA	THR	746	55.050	2.328	33.913	1.00	34.77
ATOM	5912	CB	THR	746	56.085	2.380	35.075	1.00	33.85
MOTA	5913	OG1	THR	746	56.296	1.059	35.602	1.00	33.92
MOTA	5915	CG2	THR	746	55.605	3.302	36.177	1.00	32.17
ATOM	5916	С	THR	746	55.544	1.327	32.870	1.00	32.69
ATOM	5917	0	THR	746	55.026	0.213	32.795	1.00	31.56
MOTA	5918	N	PHE	747	56.538	1.708	32.066	1.00	34.04
MOTA	5920	CA	PHE	747	57.093	0.782	31.083	1.00	31.74
ATOM	5921	CB	PHE	747	58.121	1.472	30.193	1.00	30.55
ATOM	5922	CG	PHE	747	57.504	2.287	29.096	1.00	29.40
MOTA	5923	CD1	PHE	747	56.772	1.666	28.092	1.00	28.24
MOTA	5924	CD2	PHE	747	57.609	3.667	29.091	1.00	27.50
ATOM	5925	CE1	PHE	747	56.170	2.407	27.100	1.00	24.35
ATOM	5926	CE2	PHE	747	57.001	4.413	28.091	1.00	29.27
ATOM	5927	CZ	PHE	747	56.276	3.776	27.103	1.00	25.73
				·	J J . M . U	2.,,0	-,.103	4.00	45.15

ATOM	5928	С	PHE	747	57.714	-0.413	31.782	1.00	31.92
MOTA	5929	0	PHE	747	57.727	-1.514	31.243	1.00	32.46
MOTA	5930	N	LYS	748	58.233	-0.199	32.986	1.00	33.47
MOTA	5932	CA	LYS	748	58.816	-1.302	33.733	1.00	35.57
ATOM	5933	CB	LYS	748	59.468	-0.800	35.026	1.00	39.42
ATOM	5934	CG	LYS	748	60.083	-1.923	35.861	1.00	46.49
ATOM	5935	CD	LYS	748	60.817	-1.407	37.103	1.00	50.69
MOTA	5936	CE	LYS	748	61.253	-2.574	37.999	1.00	52.57
ATOM	5937	NZ	LYS	748	62.072	-2.129	39.155	1.00	56.45
ATOM	5941	С	LYS	748	57.700	-2.318	34.028	1.00	35.58
ATOM	5942	0	LYS	748	57.898	-3.526	33.871	1.00	34.72
ATOM	5943	N	GLN	749	56.522	-1.818	34.411	1.00	35.59
MOTA	5945	CA	GLN	749	55.369	-2.684	34.692	1.00	38.20
ATOM	5946	СВ	GLN	749	54.154	-1.872	35.162	1.00	42.73
ATOM	5947	CG	GLN	749	54.264	-1.171	36.499	1.00	49.30
ATOM	5948	CD	GLN	749	53.060	-0.282	36.761	1.00	53.13
ATOM	5949	OE1	GLN	749	53.194	0.915	37.023	1.00	52.71
ATOM	5950	NE2	GLN	749	51.873	-0.856	36.644	1.00	58.54
ATOM	5953	C	GLN	749	54.954	-3.392	33.409	1.00	36.16
ATOM	5954	o	GLN	749	54.745	-4.605	33.393	1.00	36.67
ATOM	5955	N	LEU	750	54.801	-2.609	32.342	1.00	35.83
ATOM	5957	CA	LEU	750	54.381	-3.117	31.037	1.00	34.49
ATOM	5958	CB	LEU	750	54.324	-1.988	30.004	1.00	32.49
ATOM	5959	CG	LEU	750	53.206	-0.958	30.188	1.00	31.94
ATOM	5960	CD1	LEU	750	53.411	0.230	29.267	1.00	30.45
ATOM	5961	CD2	LEU	750	51.859	-1.610	29.933	1.00	29.30
ATOM	5962	C	LEU	750	55.294	-4.214	30.559	1.00	33.87
ATOM	5963	0	LEU	750	54.828	-5.208	30.027	1.00	34.72
ATOM	5964	N	VAL	751	56.598	-4.038	30.759	1.00	36.12
ATOM	5966	CA	VAL	751	57.585	-5.045	30.363	1.00	34.50
ATOM	5967	CB	VAL	751	59.054	-4.532	30.559	1.00	31.96
ATOM	5968	CG1	VAL	751	60.052	-5.646	30.308	1.00	30.24
MOTA	5969	CG2	VAL	751	59.342	-3.386	29.604	1.00	28.02
MOTA	5970	С	VAL	751	57.349	-6.321	31.182	1.00	36.11
MOTA	5971	0	VAL	751	57.333	-7.422	30.638	1.00	36.45
ATOM	5972	N	GLU	752	57.107	-6.165	32.479	1.00	37.83
MOTA	5974	CA	GLU	752	56.869	-7.326	33.331	1.00	41.47
MOTA	5975	CB	GLU	752	56.800	-6.910	34.804	1.00	43.03
MOTA	5976	CG	GLU	752	58.122	-6.305	35.263	1.00	52.52
ATOM	5977	CD	GLU	752	58.251	-6.176	36.761	1.00	57.18
MOTA	5978	OE1	GLU	752	58.600	-5.068	37.233	1.00	58.11
ATOM	5979	OE2	GLU	752	58.032	-7.191	37.461	1.00	61.59
ATOM	5980	C	GLU	752	55.623	-8.097	32.890	1.00	40.16
ATOM	5981	0	GLU	752	55.689	-9.308	32.642	1.00	39.75
ATOM	5982	N	ASP	753	54.524	-7.376	32.696	1.00	40.06
ATOM	5984	CA	ASP	753	53.275	-7.982	32.264	1.00	39.73
MOTA	5985	CB	ASP	753	52.157	-6.947	32.247	1.00	41.00
MOTA	5986	CG	ASP	753	51.668	-6.591	33.640	1.00	45.17
MOTA	5987	OD1	ASP	753	51.753	-7.468	34.543	1.00	49.78
MOTA	5988	OD2	ASP	753	51.210	-5.439	33.829	1.00	45.51
ATOM	5989	С	ASP	753	53.396	-8.595	30.890	1.00	39.64
ATOM	5990	0	ASP	753	52.955	-9.720	30.674	1.00	41.84
ATOM	5991	N	LEU	754	53.998	-7.861	29.960	1.00	37.75
MOTA	5993	CA	LEU	754	54.161	-8.358	28.603	1.00	38.16

MOTA	5994	CB	LEU	754	54.664	-7.261	27.664	1.00	36.95
MOTA	5995	CG	LEU	754	53.552	-6.270	27.307	1.00	36.64
ATOM	5996	CD1	LEU	754	54.141	-5.062	26.590	1.00	34.02
ATOM	5997	CD2	LEU	754	52.459	-6.968	26.465	1.00	34.13
MOTA	5998	С	LEU	754	55.070	-9.561	28.571	1.00	38.46
MOTA	5999	0	LEU	754	54.905	-10.451	27.740	1.00	39.95
ATOM	6000	N	ASP	755	56.014	-9.602	29.502	1.00	39.19
ATOM	6002	CA	ASP	755	56.930	-10.728	29.594	1.00	
ATOM	6003	CB	ASP	755	57.956	-10.462	30.696	1.00	40.87
ATOM	6004	CG	ASP	755	59.128	-11.415			45.11
ATOM	6005	OD1	ASP	755	59.759		30.652	1.00	48.64
ATOM	6006	OD2	ASP	755		-11.612	31.711	1.00	54.27
ATOM	6007	C	ASP	755	59.432	-11.954	29.565	1.00	51.46
ATOM	6008	0	ASP		56.082	-11.952	29.947	1.00	40.67
ATOM	6009			755	56.152	-12.996	29.289	1.00	38.49
ATOM	6011	N	ARG	756	55.232	-11.771	30.955	1.00	40.06
		CA	ARG	756	54.340	-12.817	31.437	1.00	40.07
ATOM	6012	CB	ARG	756	53.573	-12.316	32.661	1.00	40.24
ATOM	6013	CG	ARG	756	52.435	-13.217	33.138	1.00	42.12
ATOM	6014	CD	ARG	756	51.791	-12.631	34.389	1.00	42.33
ATOM	6015	NE	ARG	756	51.353	-11.247	34.186	1.00	46.68
MOTA	6017	CZ	ARG	756	50.295	-10.891	33.460	1.00	48.17
MOTA	6018	NHl	ARG	756	49.549	-11.818	32.866	1.00	46.64
MOTA	6021	NH2	ARG	756	49.998	-9.605	33.305	1.00	48.92
ATOM	6024	С	ARG	756	53.362	-13.275	30.364	1.00	40.19
MOTA	6025	0	ARG	756	53.247	-14.469	30.110	1.00	42.24
MOTA	6026	N	ILE	757	52.688	-12.327	29.717	1.00	38.18
MOTA	6028	CA	ILE	757	51.706	-12.649	28.683	1.00	38.40
ATOM	6029	CB	ILE	757	50.952	-11.382	28.187	1.00	36.55
MOTA	6030	CG2	ILE	757	49.952	-11.758	27.105	1.00	34.67
ATOM	6031	CG1	ILE	757	50.216	-10.726	29.364	1.00	34.65
ATOM	6032	CD1	ILE	757	49.554	-9.423	29.048	1.00	36.49
ATOM	6033	С	ILE	757	52.301	-13.400	27.500	1.00	39.19
ATOM	6034	0	ILE	757	51.709	-14.360	27.025	1.00	39.66
ATOM	6035	N	VAL	758	53.492	-12.996	27.061	1.00	42.36
ATOM	6037	CA	VAL	758	54.161	-13.645	25.937	1.00	43.15
MOTA	6038	CB	VAL	758	55.582	-13.052	25.682	1.00	41.72
MOTA	6039	CG1	VAL	758	56.308	-13.855	24.621	1.00	41.57
MOTA	6040	CG2	VAL	758	55.491	-11.619	25.229	1.00	40.06
MOTA	6041	C	VAL	758	54.299	-15.133	26.231	1.00	47.11
MOTA	6042	0	VAL	758	54.045	-15.971	25.369	1.00	48.62
ATOM	6043	N	ALA	759	54.695	-15.446	27.464	1.00	49.64
ATOM	6045	CA	ALA	759	54.879	-16.820	27.908	1.00	51.35
ATOM	6046	CB	ALA	759	55.423	-16.830	29.317	1.00	50.11
ATOM	6047	С	ALA	759	53.568	-17.598	27.850	1.00	54.72
ATOM	6048	0	ALA	759	53.520	-18.717	27.348	1.00	
ATOM	6049	N	LEU	760	52.496	-16.983	28.329		58.64
ATOM	6051	CA	LEU	760	51.194	-17.628		1.00	54.84
ATOM	6052	СВ	LEU	760	50.330	-17.028	28.343	1.00	55.87
ATOM	6053	CG	LEU	760	50.330		29.459	1.00	56.85
ATOM	6054	CD1	LEU	760		-17.165 -16.302	30.885	1.00	56.80
ATOM	6055	CD2	LEU	760	49.991	-16.392	31.849	1.00	56.78
ATOM	6056	CD2			50.959	-18.631	31.289	1.00	57.78
			LEU	760	50.454	-17.546	27.013	1.00	57.36
ATOM	6057	0	LEU	760	49.262	-17.859	26.944	1.00	57.65
ATOM	6058	N	THR	761	51.151	-17.134	25.956	1.00	58.71

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MOTA 6060 CA THR 761 -17.025 24.630 1.00 59.04 50.541 MOTA 6061 CB THR 761 23.971 50.839 -15.657 1.00 56.72 -14.610 ATOM 6062 OG1 THR 761 50.287 24.775 1.00 56.53 MOTA 6064 CG2 761 THR 50.213 -15.584 22.590 1.00 53.81 MOTA 6065 С THR 761 51.049 -18.138 23.721 1.00 60.44 MOTA 6066 THR 761 0 52.255 -18.295 23.530 1.00 61.40 MOTA 6067 SG CYS 1603 18.474 -8.976 20.202 0.50 37.82 PRT2 MOTA 6068 CG MET 534 69.311 12.109 23.281 0.50 36.25 PRT2 6069 0.50 42.66 PRT2 MOTA SD MET 534 69.286 12.958 24.867 MOTA 6070 CE MET 12.083 25.804 0.50 43.27 PRT2 534 70.539 MOTA -7.949 16.446 0.50 36.47 PRT2 6071 SG CYS 603 56.046 MOTA 2676 TIP3 1 25.061 1.00 24.53 OH2 71.794 2.660 MOTA 2679 1.00 39.62 OH2 TIP3 2 39.750 3.992 15.898 19.717 10.596 MOTA 2682 OH2 TIP3 3 83.809 1.00 28.26 7.685 1.00 26.19 MOTA 2685 OH2 TIP3 4 83.630 20.056 ATOM 2688 OH2 TIP3 5 75.073 16.616 6.785 1.00 26.48 MOTA 2691 OH2 TIP3 6 86.549 19.594 9.502 1.00 33.65 MOTA TIP3 7 2694 OH2 51.913 11.060 24.263 1.00 35.55 ATOM 2697 TIP3 8 OH2 55.093 9.421 22.524 1.00 26.63 ATOM 2700 OH2 TIP3 9 57.161 4.614 32.443 1.00 29.69 MOTA 2703 OH2 TIP3 10 52.169 4.735 13.281 1.00 22.61 MOTA 2706 41.110 5.543 22.764 1.00 41.60 OH2 TIP3 11 45.145 8.857 21.555 1.00 36.99 MOTA 2709 OH2 TIP3 12 ATOM 2712 64.465 -2.607 28.883 1.00 30.17 OH2 TIP3 13 ATOM 2715 76.944 13.287 23.954 1.00 32.94 OH2 TIP3 14 MOTA 2718 OH2 TIP3 15 79.062 17.048 18.200 1.00 51.65 MOTA 2721 OH2 TIP3 16 83.066 11.657 15.958 1.00 25.12 MOTA 2724 OH2 TIP3 17 13.957 -9.951 0.095 1.00 26.02 MOTA 2727 OH2 TIP3 18 38.359 -0.001 5.000 1.00 37.43 MOTA 2730 OH2 TIP3 19 5.442 2.705 19.077 1.00 29.46 ATOM 2733 OH2 TIP3 20 27.008 6.166 4.885 1.00 25.05 MOTA TIP3 21 2736 OH2 34.242 -1.725 16.911 1.00 52.12 ATOM 2739 OH2 TIP3 22 20.167 2.428 27.681 1.00 42.69 ATOM 2742 OH2 TIP3 23 50.794 -11.834 38.045 1.00 60.16 MOTA 2745 OH2 TIP3 24 1.00 25.88 17.261 -5.993 -1.757 MOTA 2748 OH2 TIP3 25 1.00 39.33 27.516 7.803 15.070 MOTA 2751 OH2 TIP3 26 31.574 0.146 6.684 1.00 35.78 ATOM 2754 OH2 TIP3 27 27.119 -12.972 27.844 1.00 43.66 MOTA 2757 OH2 TIP3 28 28.439 -17.074 13.203 1.00 36.44 MOTA 2760 OH2 TIP3 29 88.706 14.393 7.969 1.00 32.49 MOTA 2763 -3.424 OH2 TIP3 30 -2.338 11.295 1.00 49.20 ATOM 2766 OH2 TIP3 31 35.086 -4.130 18.836 1.00 37.83 ATOM 2769 TIP3 32 80.455 OH2 17.922 9.507 1.00 23.69 ATOM 2772 OH2 TIP3 33 5.538 3.619 10.835 1.00 29.13 ATOM 2775 OH2 TIP3 34 -10.685 5.290 11.288 1.00 24.40 ATOM 2778 OH2 TIP3 35 29.210 -8.799 20.241 1.00 46.52 MOTA 2781 OH2 TIP3 36 6.195 3.150 13.803 1.00 31.39 MOTA 2784 TIP3 37 OH2 31.898 2.830 0.154 1.00 40.17 ATOM 2787 OH2 TIP3 38 19.915 2.023 1.00 31.34 -3.939 MOTA 2790 OH2 TIP3 39 2.604 62.242 32.859 1.00 39.67 MOTA 2793 TIP3 40 OH2 21.231 -7.063 -3.900 1.00 23.55 ATOM 2796 OH2 TIP3 41 8.838 22.610 -15.809 1.00 36.02 MOTA 2799 OH2 TIP3 42 40.120 2.154 8.433 1.00 60.62 MOTA 2802 OH2 TIP3 43 19.583 11.128 -0.045 1.00 37.85

ATOM	2805	OH2	TIP3	44	67.056	9.030	17 200	3 00	20.70
ATOM	2808	OH2	TIP3	45	87.772	18.919	17.389	1.00	29.79
ATOM	2811	OH2	TIP3	46	74.584	17.123	18.595	1.00	48.44
ATOM	2814	OH2	TIP3	47			4.200	1.00	39.18
ATOM	2817	OH2	TIP3	48	29.365	16.707	10.560	1.00	34.11
ATOM	2820	OH2	TIP3	49	66.486	6.826	15.051	1.00	32.28
ATOM	2823	OH2			85.008	21.441	5.731	1.00	23.97
ATOM	2826	OH2	TIP3	50	-4.572	2.912	3.173	1.00	28.05
ATOM			TIP3	51	19.496	5.141	4.881	1.00	28.88
ATOM	2829	OH2	TIP3	52	67.492	3.490	10.902	1.00	33.57
	2832	OH2	TIP3	53	34.791	5.413	24.797	1.00	40.16
ATOM	2835	OH2	TIP3	54	34.787	-16.910	13.756	1.00	39.46
ATOM	2838	OH2	TIP3	55	59.972	7.450	27.870	1.00	31.56
ATOM	2841	OH2	TIP3	56	-7.139	-1.696	6.345	1.00	42.00
ATOM	2844	OH2	TIP3	57	54.998	11.953	25.360	1.00	42.05
ATOM	2847	OH2	TIP3	58	68.697	6.686	16.740	1.00	46.12
ATOM	2850	OH2	TIP3	59	73.750	20.885	19.041	1.00	32.26
ATOM	2853	OH2	TIP3	60	3.431	-8.270	-8.218	1.00	31.22
ATOM	2856	OH2	TIP3	61	37.904	10.790	5.612	1.00	33.72
ATOM	2859	OH2		62	29.982	-9.545	~1.303	1.00	39.11
ATOM	2862	ОН2	TIP3	63	66.918	1.757	8.678	1.00	34.68
MOTA	2865	OH2	TIP3	64	49.117	1.310	12.227	1.00	34.31
MOTA	2868	OH2	TIP3	65	41.246	3.987	29.033	1.00	34.55
ATOM	2871	OH2	TIP3	66	10.755	-12.957	1.167	1.00	42.14
ATOM	2874	OH2	TIP3	67	-1.184	-4.327	21.439	1.00	37.90
ATOM	2877	OH2	TIP3		30.349	16.267	13.265	1.00	55.23
ATOM	2880	OH2	TIP3	69	8.111	4.362	3.445	1.00	23.88
ATOM	2883	OH2	TIP3	70	73.131	18.780	22.628	1.00	40.20
MOTA	2886	OH2	TIP3	71	-7.949	-3.409	24.953	1.00	35.49
ATOM	2889	OH2	TIP3	72	66.379	-4.621	28.423	1.00	45.46
ATOM	2892	OH2	TIP3	73	21.506	-20.711	4.815	1.00	52.46
ATOM	2895	OH2	TIP3	74	59.539	-6.865	4.928	1.00	48.87
ATOM	2898	OH2	TIP3	75	16.565	-13.297	-3.008	1.00	51.80
MOTA	2901	OH2	TIP3	76	-15.235	7.385	4.428	1.00	29.13
MOTA	2904	OH2	TIP3	77	32.926	2.785	13.213	1.00	37.62
ATOM	2907	OH2	TIP3	78	0.246	-2.768	10.996	1.00	28.25
ATOM	2910	OH2	TIP3	79	17.495	2.354	5.447	1.00	23.63
MOTA	2913	OH2	TIP3	80	6.336	2.434	21.950	1.00	29.56
MOTA	2916	OH2	TIP3	81	27.374	3.628	6.163	1.00	34.06
MOTA	2919	OH2	TIP3	82	-8.708	6.263	9.522	1.00	30.34
ATOM	2922	OH2	TIP3	83	1.500	-1.935	8.721	1.00	27.61
ATOM	2925	OH2	TIP3	84	-4.825	-3.133	6.984	1.00	33.50
ATOM	2928	OH2	TIP3	85	17.513	2.839	1.966	1.00	24.27
MOTA	2931	OH2	TIP3	86	20.298	3.414	2.920	1.00	26.15
ATOM	2934	OH2	TIP3	87	0.488	-2.158	22.213	1.00	25.95
MOTA	2937	OH2	TIP3	88	19.939	-6.185	-1.553	1.00	19.14
MOTA	2940	OH2	TIP3	89	10.670	-15.654	6.839	1.00	33.36
ATOM	2943	OH2	TIP3	90	4.107	-12.003	11.805	1.00	33.92
ATOM	2946	OH2	TIP3	91	6.238	0.927	-3.342	1.00	23.31
MOTA	2949	OH2	TIP3	92	-13.563	1.438	5.472	1.00	27.86
MOTA	2952	OH2	TIP3	93	15.707	-7.454	0.106	1.00	26.69
ATOM	2955	OH2	TIP3	94	-1.856	-5.393	3.795	1.00	39.91
ATOM	2958	OH2	TIP3		12.654	4.928	-4.474	1.00	31.32
ATOM	2961	OH2	TIP3		69.774	27.363	2.127	1.00	35.86
ATOM	2964	OH2	TIP3		24.636	-13.192	0.040	1.00	48.53
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MOTA	2967	OH2	TIP3	98	60.453	-4.625	33.829	1.00	31.97
MOTA	2970	ОН2	TIP3	99	10.513	5.719	3.487	1.00	
MOTA	2973	OH2	TIP3	100	-9.499	-4.011	4.342	1.00	30.61
ATOM	2976	OH2	TIP3	101	73.056	-1.608	10.514	1.00	36.08
ATOM	2979	OH2	TIP3	102	-3.152	5.709	30.608	1.00	29.38
ATOM	2982	OH2	TIP3	103	36.630	0.702	11.792	1.00	47.80
ATOM	2985	OH2	TIP3	104	21.475	6.325	16.924	1.00	24.03
ATOM	2988	OH2	TIP3	105	31.272	0.656	19.432	1.00	53.74
MOTA	2991	OH2	TIP3	106	5.620	-8.417	22.266	1.00	51.90
ATOM	2994	OH2	TIP3	107	-13.144	8.294	17.464	1.00	35.23
ATOM	2997	OH2	TIP3	108	26.680	-10.556	-1.042	1.00	27.83
ATOM	3000	OH2	TIP3	109	24.149	1.846	18.172	1.00	30.90
ATOM	3003	OH2	TIP3	110	-1.943	12.643	3.558	1.00	33.82
ATOM	3006	OH2	TIP3	111	59.560	13.617	33.196	1.00	54.79
ATOM	3009	OH2	TIP3		4.351	-10.740	1.991	1.00	37.96
ATOM	3012	OH2	TIP3		8.396	2.913	0.958	1.00	29.64
ATOM	3015	OH2	TIP3		75.905	1.753	25.812	1.00	38.73
ATOM	3018	OH2	TIP3		48.783	15.535	14.189	1.00	35.24
ATOM	3021	OH2		116	2.419	-11.312	9.146	1.00	
ATOM	3024	OH2		117	83.014	26.360	12.964	1.00	32.85 41.83
ATOM	3027	OH2		118	8.761	-6.579	-3.252	1.00	42.78
MOTA	3030	OH2		119	-8.417	4.493	4.305	1.00	28.32
ATOM	3033	OH2	TIP3		7.908	~13.690	8.639	1.00	33.73
ATOM	3036	OH2	TIP3		51.437	6.329	10.373	1.00	31.72
ATOM	3039	OH2	TIP3		20.660	3.686	15.591	1.00	32.37
ATOM	3042	OH2	TIP3		73.039	3.790	20.450	1.00	35.80
ATOM	3045	OH2	TIP3		5.155	-11.467	22.590	1.00	45.12
ATOM	3048	OH2	TIP3		34.172	2.412	16.576	1.00	41.90
ATOM	3051	OH2		126	9.597	-11.905	7.083	1.00	24.83
MOTA	3054	OH2		127	8.276	3.860	-1.622	1.00	35.46
ATOM	3057	OH2	TIP3		66.282	5.755	12.352	1.00	35.43
ATOM	3060	OH2	TIP3	129	7.377	6.932	2.982	1.00	40.68
ATOM	3063	OH2	TIP3	130	35.832	-1.778	0.201	1.00	34.99
MOTA	3066	OH2	TIP3	131	44.781	10.362	11.064	1.00	42.31
ATOM	3069	OH2	TIP3	132	27.790	-12.638	18.958	1.00	58.71
ATOM	3072	OH2	TIP3	133	45.221	11.540	21.428	1.00	36.75
MOTA	3075	OH2	TIP3	134	57.560	-10.846	14.099	1.00	52.90
MOTA	3078	OH2	TIP3	135	-3.354	15.001	16.515	1.00	37.81
ATOM	3081	OH2	TIP3	136	85.717	11.251	9.062	1.00	35.18
MOTA	3084	OH2	TIP3	137	12.951	-2.469	2.075	1.00	22.07
MOTA	3087	ОН2	TIP3	138	75.645	3.486	20.527	1.00	38.01
MOTA	3090	OH2	TIP3	L39	13.237	7.412	-2.649	1.00	33.50
MOTA	3093	OH2	TIP3	L40	11.262	-9.970	0.974	1.00	26.14
MOTA	3096	OH2	TIP3	141	59.480	10.772	14.098	1.00	52.08
ATOM	3099	OH2	TIP3	L42	13.869	-16.121	3.919	1.00	40.06
ATOM	3102	OH2	TIP3	143	-6.407	-3.413	16.641	1.00	44.38
ATOM	3105	ОН2	TIP3	144	25.667	-12.645	3.411	1.00	48.28
MOTA	3108	OH2	TIP3		-16.282	10.641	6.423	1.00	40.94
MOTA	3111	OH2	TIP3 1		B6.637	12.861	7.008	1.00	39.45
ATOM	3114	ОН2	TIP3 1		32.082	-4.569	1.892	1.00	27.35
ATOM	3117	OH2	TIP3 1		44.809	7.627	11.670	1.00	35.65
MOTA	3120	OH2	TIP3 1		80.693	12.459	16.523	1.00	37.21
MOTA	3123	OH2	TIP3 1		2.941	-7.118	-1.805	1.00	38.43
ATOM	3126	OH2		.51	31.794	-6.086	20.704	1.00	42.80
						9.000	20.704	00	74.DU

MOTA	3129	OH2	TIP3	152	74.770	-2.683	12.398	1.00	40.40
ATOM	3132	OH2	TIP3	153	7.731	6.640	-1.037	1.00	35.61
ATOM	3135	OH2	TIP3	154	71.617	5.599	21.838	1.00	40.14
MOTA	3138	OH2	TIP3	155	68.113	-4.968	8.886	1.00	34.38
MOTA	3141	OH2	TIP3	156	0.042	-9.364	7.055	1.00	33.08
MOTA	3144	OH2	TIP3	157	68.020	18.352	10.995	1.00	34.76
MOTA	3147	OH2	TIP3	158	3.795	8.550	4.533	1.00	34.69
MOTA	3150	OH2	TIP3	159	52.106	11.746	18.410	1.00	40.06
MOTA	3153	OH2	TIP3	160	6.414	3.927	16.889	1.00	37.07
MOTA	3156	OH2	TIP3	161	-10.282	6.603	4.715	1.00	38.48
ATOM	3159	OH2	TIP3	162	76.410	1.681	-0.781	1.00	42.87
MOTA	3162	OH2	TIP3	163	9.910	-12.046	17.157	1.00	32.79
ATOM	3165	OH2	TIP3	164	33.983	14.219	18.191	1.00	37.35
MOTA	3168	OH2	TIP3	165	2.330	-7.952	16.978	1.00	44.25
MOTA	3171	OH2	TIP3	166	29.701	1.780	5.987	1.00	39.86
ATOM	3174	OH2	TIP3	167	32.494	-17.319	11.798	1.00	38.46
MOTA	3177	OH2	TIP3	168	42.107	17.932	10.978	1.00	44.83
ATOM	3180	OH2	TIP3	169	87.822	10.537	5.568	1.00	54.30
MOTA	3183	OH2	TIP3	170	70.261	-4.143	25.064	1.00	44.75
MOTA	3186	OH2	TIP3	171	77.519	5.882	23.891	1.00	42.67
MOTA	3189	OH2	TIP3	172	-0.921	-8.166	4.521	1.00	45.91
ATOM	3192	OH2	TIP3	173	34.213	15.329	1.478	1.00	40.10
ATOM	3195	OH2		174	-9.647	7.731	7.383	1.00	35.63
ATOM	3198	ОН2	TIP3	175	11.619	5.799	7.440	1.00	36.36
ATOM	3201	OH2		176	-8.709	13.964	13.507	1.00	51.97
ATOM	3204	OH2	TIP3	177	31.770	3.376	18.354	1.00	46.26
ATOM	3207	OH2	TIP3	178	-8.494	9.789	24.269	1.00	50.98
MOTA	3210	OH2	TIP3	179	-1.234	-6.253	15.622	1.00	38.47
MOTA	3213	OH2	TIP3		80.252	0.887	15.691	1.00	39.48
MOTA	3216	OH2	TIP3		67.248	20.272	-1.555	1.00	48.22
ATOM	3219	OH2	TIP3	182	-0.566	4.367	1.362	1.00	39.84
ATOM	3222	OH2	TIP3		0.120	6.523	2.615	1.00	33.11
MOTA	3225	OH2	TIP3	184	-1.496	8.789	1.237	1.00	41.03
ATOM	3228	OH2	TIP3	185	-5.143	9.130	2.236	1.00	40.47
ATOM	3231	OH2	TIP3	186	-7.275	10.106	3.833	1.00	40.55
ATOM	3234	OH2	TIP3	187	2.717	7.275	0.769	1.00	44.67
ATOM	3237	OH2	TIP3	188	5.176	10.645	8.459	1.00	34.48
ATOM	3240	OH2	TIP3	189	63.822	12.690	22.883	1.00	41.88
MOTA	3243	OH2		190	79.109	1.028	18.201	1.00	46.40
ATOM	3246	OH2	TIP3		59.332	-11.681	7.236	1.00	63,45
ATOM	3249	OH2	TIP3		13.967	-1.218	-4.268	1.00	34.79
MOTA	3252	OH2	TIP3		59.444	2.867	33.368	1.00	41.00
ATOM	3255	OH2	TIP3		32.024	13.487	19.852	1.00	53.61
ATOM	3258	OH2	TIP3		72.101	16.218	22.802	1.00	44.03
ATOM	3261	OH2	TIP3		0.987	-8.546	14.474	1.00	41.38
ATOM	3264	OH2	TIP3		-0.491	5.461	30.372	1.00	38.51
ATOM	3267	OH2	TIP3		61.179	6.795	11.905	1.00	41.77
ATOM	3270	OH2	TIP3		-1.365	-4.128	27.656	1.00	50.98
ATOM	3273	OH2	TIP3		81.440	15.558	17.262	1.00	44.47
ATOM	3276	OH2	TIP3		-17.491	4.116	23.873	1.00	50.58
ATOM	3279	OH2	TIP3		27.546	10.513	14.499	1.00	39.06
ATOM	3282	OH2	TIP3		34.992	4.513	27.719	1.00	
ATOM	3285	OH2	TIP3		-3.486	-4.513 -4.591	9.171	1.00	49.89
ATOM	3288	OH2	TIP3		42.799	7.848	22.320		49.53
444011	2200	OHZ	ALFS	203	74.133	7.040	22.320	1.00	43.50

ATOM	3291	OH2	TIP3 206	52.728	11.884	21.811	1.00	39.98
MOTA	3294	OH2	TIP3 207	26.706	14.069	19.833	1.00	46.68
MOTA	3297	OH2	TIP3 208	-7.154	8.907	6.444	1.00	42.83
ATOM	3300	OH2	TIP3 209	86.648	5.606	16.034	1.00	51.15
ATOM	3303	OH2	TIP3 210	54.879	15.840	20.379	1.00	50.23
ATOM	3306	OH2	TIP3 211	51.417	19.473	22.691	1.00	48.35
ATOM	3309	OH2	TIP3 212	20.102	6.924	7.085	1.00	38.15
ATOM	3312	OH2	TIP3 213	28.991	1.941	-3.570	1.00	47.39
ATOM	3315	OH2	TIP3 214	26.505	2.386	-4.633	1.00	46.48
MOTA	3318	OH2	TIP3 215	36.482	2.810	18.521	1.00	46.26
MOTA	3321	OH2	TIP3 216	16.941	-20.504	14.128	1.00	49.74
MOTA	3324	OH2	TIP3 217	28.572	-14.448	6.157	1.00	49.13
MOTA	3327	OH2	TIP3 218	31.380	1.471	-1.998	1.00	43.02
MOTA	3330	OH2	TIP3 219	10.065	-16.338	15.455	1.00	42.75
ATOM	3333	OH2	TIP3 220	7.350	-11.974	5.652	1.00	55.35
ATOM	3336	OH2	TIP3 221	-12.328	14.547	10.986	1.00	51.29
MOTA	3339	OH2	TIP3 222	11.186	9.609	-1.388	1.00	37.68
ATOM	3342	OH2	TIP3 223	11.389	12.276	-1.400	1.00	46.93
ATOM	3345	OH2	TIP3 224	34.202	13.069	-1.161	1.00	41.79
MOTA	3348	OH2	TIP3 225	31.303	17.822	7.853	1.00	48.21
ATOM	3351	OH2	TIP3 226	36.875	11.804	-2.106	1.00	59.03
ATOM	3354	OH2	TIP3 227	35.134	3.048	11.020	1.00	50.41
ATOM	3357	OH2	TIP3 228	63.950	13.409	26.627	1.00	43.40
ATOM	3360	OH2	TIP3 229	36.367	6.116	15.221	1.00	57.79
ATOM	3363	OH2	TIP3 230	90.606	4.355	6.342	1.00	47.53
ATOM	3366	OH2	TIP3 231	50.038	-11.673	10.767	1.00	56.90
MOTA	3369	OH2	TIP3 232	60.196	-10.144	16.590	1.00	51.61
ATOM	3372	OH2	TIP3 233	18.021	-21.179	7.008	1.00	49.93
ATOM	3375	OH2	TIP3 234	66.236	-1.218	30.583	1.00	39.55
MOTA	3378	OH2	TIP3 235	74.959	18.928	20.659	1.00	38.04
ATOM	3381	OH2	TIP3 236	2.816	10.082	3.187	1.00	49.31
ATOM	3384	OH2	TIP3 237	5.894	-3.410	25.289	1.00	35.55
ATOM ATOM	3387	OH2	TIP3 238	35.784	6.047	12.543	1.00	41.96
ATOM	3390 3393	OH2 OH2	TIP3 239 TIP3 240	-5.400	16.537	14.180	1.00	43.13
MOTA	3396	OH2	TIP3 240	46.589	-11.622	26.970	1.00	43.71
ATOM	3399	OH2	TIP3 241	6.199	6.592	13.797	1.00	46.51
ATOM	3402	OH2	TIP3 242	-3.777 1.969	-5.158	20.907	1.00	42.08
ATOM	3405	OH2	TIP3 243	86.200	-3.711 11.629	-0.282	1.00	37.38
ATOM	3408	OH2	TIP3 244	10.557	7.565	22.877	1.00	56.51
ATOM	3411	OH2	TIP3 245	4.802	8.149	5.514 2.136	1.00	47.58
ATOM	3414	OH2	TIP3 247	64.590	-8.128	20.596	1.00	50.70
ATOM	3417	OH2	TIP3 248	11.346	-17.840	13.283	1.00	43.65
ATOM	3420	OH2	TIP3 249	42.116	-6.808	14.953	1.00	47.64
ATOM	3423	OH2	TIP3 250	2.745	-4.054	22.128		53.79
ATOM	3426	OH2	TIP3 251	71.999	1.177		1.00	60.88
ATOM	3429	OH2	TIP3 251	50.328	-3.210	-2.124 33.068	1.00	47.90
ATOM	3435	OH2	TIP3 252	57.838	9.337	11.631	1.00	57.01
ATOM	3438	OH2	TIP3 253	43.373	20.489	30.490	1.00	52.55
MOTA	3441	OH2	TIP3 255	67.045	16.529	15.793	1.00	51.97
ATOM	3444	OH2	TIP3 256	87.509	21.566	5.114	1.00	49.02
ATOM	3447	OH2	TIP3 257	21.060	10.052	-9.215	1.00	54.21
ATOM	3450	OH2	TIP3 258	11.827	2.450	27.951	1.00	60.32 54.26
ATOM	3453	OH2	TIP3 259	64.788	-0.418	3.563	1.00	
				04.700	0.410	J.JOJ	1.00	50.94

202

MOTA	3456	OH2	TIP3	260	71.859	28.473	7.950	1.00	62.81
ATOM	3459	OH2	TIP3	261	25.605	-8.106	27.287	1.00	52.81
MOTA	3462	OH2	TIP3	262	-18.804	10.886	12.628	1.00	55.25
MOTA	3465	OH2	TIP3	263	30.652	11.349	16.201	1.00	50.40
MOTA	3468	OH2	TIP3	264	22.350	-16.098	-2.742	1.00	53.27
ATOM	3471	OH2	TIP3	265	29.720	9.106	18.465	1.00	57.23

203

TABLE 2

2+		34			v	v	a	000	
Atom		Atom	A.A	A.A	Х	Y	Z	occ	В
No.		Туре	Type	No.	13 435	16 262	0 075	3 00	61 21
ATOM	1	N	GLU	1464	-13.425	16.769	8.973	1.00	61.21
ATOM	3	CA	GLU	1464	-12.536	16.852	7.821	1.00	59.70
MOTA	4	СВ	GLU	1464	-11.383	17.829	8.085	1.00	60.05
MOTA	5	С	GLU	1464	-11.998	15.478	7.427	1.00	57.11
ATOM	6	0	GLU	1464	-12.134	15.076	6.274	1.00	59.75
MOTA	7	N	LEU	1465	-11.406	14.749	8.368	1.00	52.21
ATOM	9	CA	LEU	1465	-10.871	13.424	8.062	1.00	46.72
MOTA	10	CB	LEU	1465	-10.102	12.844	9.249	1.00	44.98
MOTA	11	CG	LEU	1465	-8.608	13.123	9.384	1.00	46.11
MOTA	12	CD1	LEU	1465	-8.338	14.592	9.663	1.00	51.13
MOTA	13	CD2	LEU	1465	-8.064	12.286	10.512	1.00	4.99
MOTA	14	С	LEU	1465	-12.000	12.475	7.700	1.00	44.16
ATOM	15	0	LEU	1465	-13.101	12.577	8.239	1.00	44.04
MOTA	16	N	PRO	1466	-11.760	11.580	6.732	1.00	42.53
MOTA	17	CD	PRO	1466	-10.535	11.534	5.913	1.00	41.30
ATOM	18	CA	PRO	1466	-12.740	10.591	6.269	1.00	41.16
ATOM	19	CB	PRO	1466	-12.134	10.111	4.959	1.00	41.48
ATOM	20	CG	PRO	1466	-10.658	10.213	5.220	1.00	41.30
ATOM	21	С	PRO	1466	-12.906	9.441	7.261	1.00	41.31
MOTA	22	0	PRO	1466	-11.929	8.936	7.816	1.00	41.05
MOTA	23	N	GLU	1467	-14.145	9.044	7.500	1.00	41.02
MOTA	25	CA	GLU	1467	-14.428	7.960	8.427	1.00	42.42
MOTA	26	CB	GLU	1467	-15.931	7.904	8.712	1.00	47.98
MOTA	27	CG	GLU	1467	-16.565	9.238	9.105	1.00	52.79
ATOM	28	CD	GLU	1467	-17.998	9.093	9.606	1.00	54.21
MOTA	29	OE1	GLU	1467	-18.474	7.949	9.741	1.00	58.90
MOTA	30	OE2	GLU	1467	-18.650	10.120	9.879	1.00	55.90
MOTA	31	С	GLU	1467	-13.972	6.628	7.837	1.00	40.93
MOTA	32	0	GLU	1467	-14.061	6.426	6.620	1.00	44.32
ATOM	33	N	ASP	1468	-13.473	5.731	8.689	1.00	35.10
ATOM	35	CA	ASP	1468	-13.024	4.404	8.256	1.00	31.82
MOTA	36	CB	ASP	1468	-11.507	4.358	7.992	1.00	30.65
MOTA	37	CG	ASP	1468	-11.025	3.002	7.440	1.00	29.93
ATOM	38	OD1	ASP	1468	-11.689	1.958	7.603	1.00	29.63
ATOM	39	OD2	ASP	1468	-9.945	2.974	6.835	1.00	33.63
MOTA	40	С	ASP	1468	-13.394	3.441	9.369	1.00	31.81
MOTA	41	0	ASP	1468	-12.618	3.209	10.302	1.00	31.91
ATOM	42	N	PRO	1469	-14.569	2.819	9.247	1.00	29.68
ATOM	43	CD	PRO	1469	-15.482	2.963	8.097	1.00	28.33
ATOM	44	CA	PRO	1469	-15.100	1.863	10.220	1.00	31.80
MOTA	45	CB	PRO	1469	-16.352	1.331	9.510	1.00	32.51
ATOM	46	CG	PRO	1469	-16.783	2.496	8.656	1.00	27.41
MOTA	47	С	PRO	1469	-14.146	0.731	10.590	1.00	30.44
ATOM	48	0	PRO	1469	-14.272	0.135	11.654	1.00	30.02
ATOM	49	N	ARG	1470	-13.198	0.442	9.704	1.00	31.06
ATOM	51	CA	ARG	1470	-12.240	-0.636	9.917	1.00	31.86
ATOM	52	CB	ARG	1470	-11.386	-0.860	8.660	1.00	31.36
ATOM	53	CG	ARG	1470	-12.107	-1.437	7.448	1.00	33.08

MOTA 54 ,CD ARG 1470 -11.148 -1.588 6.248 1.00 31.08 **ATOM** 55 NE ARG 1470 -10.540 -0.310 5.891 1.00 34.36 MOTA 57 CZARG 1470 -9.656 -0.135 4.919 1.00 33.32 MOTA 58 NH1 ARG 1470 -9.260 -1.164 4.185 1.00 35.90 MOTA 61 NH₂ ARG 1470 -9.155 1.074 4.687 1.00 32.79 MOTA 64 С ARG 1470 -11.290 -0.436 11.095 1.00 32.68 MOTA 65 0 ARG 1470 -10.820 -1.410 11.683 1.00 33.43 **ATOM** 66 N TRP 1471 -11.031 0.814 11.456 1.00 31.84 MOTA 68 CA TRP 1471 -10.063 1.090 12.505 1.00 31.17 MOTA 69 CB TRP 1471 -8.816 1.677 11.850 1.00 30.15 **ATOM** 70 CG TRP 1471 -8.173 0.725 10.941 1.00 29.54 MOTA 71 CD2 TRP 1471 -7.288 -0.329 11.315 1.00 31.07 MOTA 72 CE₂ TRP 1471 -6.913 -0.992 10.132 1.00 34.41 **ATOM** 73 CE3 TRP 1471 -6.762 -0.76B 12.536 1.00 29.46 ATOM 74 CD1 TRP 1471 -8.309 0.660 9.587 1.00 30.20 **ATOM** 75 NE1 TRP 1471 -7.557 -0.3719.089 1.00 33.09 **ATOM** 77 CZ2 TRP 1471 -6.042 ~2.085 10.135 1.00 31.68 **ATOM** 78 CZ3 TRP 1471 -5.897 -1.853 12.540 1.00 29.65 **ATOM** 79 CH2 TRP 1471 -5.541 -2.494 11.347 1.00 30.18 MOTA 80 C TRP 1471 -10.477 2.019 13.620 1.00 29.94 MOTA 81 O TRP 1471 -9.782 2.108 14.631 1.00 30.00 MOTA 82 N GLU 1472 -11.573 2.737 13.416 1.00 29.06 MOTA 84 CA GLU 1472 -12.051 3.706 14.380 1.00 28.62 MOTA 85 CB GLU 1472 -13.312 4.386 13.849 1.00 29.16 **MOTA** 86 CG GLU 1472 -13.641 5.733 14.529 1.00 30.74 **MOTA** 87 CD GLU 1472 -12.676 6.848 14.156 1.00 30.05 MOTA 88 OEl GLU 1472 -12.090 6.799 13.057 1.00 31.32 MOTA 89 OE2 GLU 1472 -12.511 7.784 14.961 1.00 30.26 MOTA 90 C GLU 1472 -12.327 3.159 15.767 1.00 28.70 MOTA 91 0 GLU 1472 -12.969 2.125 15.916 1.00 31.01 **ATOM** 92 N LEU 1473 -11.810 3.842 16.781 1.00 27.38 **ATOM** 94 LEU 1473 CA -12.054 3.451 18.161 1.00 29.61 **ATOM** 95 CB LEU 1473 -10.763 3.073 18.899 1.00 28.56 **ATOM** 96 CG LEU 1473 -10.9232.756 20.403 1.00 30.06 **ATOM** 97 CD1 LEU 1473 -11.485 1.354 20.639 1.00 28.42 MOTA 98 CD2 LEU 1473 -9.595 2.876 21.115 1.00 28.15 MOTA 99 C LEU 1473 -12.617 4.714 18.764 1.00 31.81 **ATOM** 100 0 LEU 1473 -12.1795.814 18.407 1.00 33.00 MOTA 101 N **PRO** 1474 -13.670 4.591 19.596 1.00 31.45 **ATOM** 102 CD **PRO** 1474 -14.4883.400 19.859 1.00 31.72 **ATOM** 103 CA **PRO** 1474 -14.261 5.774 20.226 1.00 31.23 **MOTA** 104 CB **PRO** 1474 -15.400 5.176 21.048 1.00 29.01 **ATOM** 105 CG PRO 1474 -15.815 4.005 20.247 1.00 29.09 MOTA 106 C PRO 1474 -13.217 6.444 21.120 1.00 33.36 **ATOM** 107 O PRO 1474 -12.447 5.765 21.808 1.00 36.40 **ATOM** 108 N ARG 1475 -13.188 7.770 21.112 1.00 33.67 MOTA 110 CA ARG 1475 -12.228 8.498 21.924 1.00 33.96 **ATOM** 111 CB ARG 1475 -12.433 9.991 21.735 1.00 35.31 MOTA 112 CG ARG 1475 -12.134 10.405 20.333 1.00 40.10 **ATOM** 113 CD ARG 1475 -12.060 11.906 20.145 1.00 42.98 ATOM 114 NE ARG 1475 -11.785 12.194 18.737 1.00 42.91 MOTA 116 CZ. ARG 1475 -10.578 12.443 18.253 1.00 41.30 MOTA 117 NH₃ ARG 1475 -9.529 12.467 19.064 1.00 41.88 **ATOM** 120 NH2 1475 ARG -10.413 12.567 16.943 1.00 40.98

ATOM	123	С	ARG	1475	-12.278	8.142	23.404	1.00	35.88
ATOM	124	0	ARG	1475	-11.240	8.046	24.061	1.00	37.10
MOTA	125	N	ASP	1476	-13.479	7.920	23.928	1.00	36.47
MOTA	127	CA	ASP	1476	-13.632	7.581	25.335	1.00	37.24
ATOM	128	CB	ASP	1476	-15.112	7.629	25.741	1.00	39.66
ATOM	129	CG	ASP	1476	-15.930	6.480	25.163	1.00	42.38
ATOM	130	OD1	ASP	1476	-15.438	5.706	24.322	1.00	47.52
ATOM	131	OD2	ASP	1476	-17.098	6.349	25.568	1.00	48.06
ATOM	132	С	ASP	1476	-13.023	6.232	25.724	1.00	36.93
MOTA	133	0	ASP	1476	-13.034	5.856	26.898	1.00	40.09
MOTA	134	N	ARG	1477	-12.564	5.475	24.732	1.00	34.34
ATOM	136	CA	ARG	1477	-11.961	4.171	24.993	1.00	32.47
ATOM	137	CB	ARG	1477	-12.269	3.212	23.852	1.00	31.59
ATOM	138	CG	ARG	1477	-13.716	2.939	23.640	1.00	29.66
MOTA	139	CD	ARG	1477	-14.314	2.342	24.875	1.00	30.65
ATOM	140	NE	ARG	1477	-14.498	3.342	25.918	1.00	31.37
ATOM	142	CZ	ARG	1477	-14.822	3.055	27.174	1.00	32.81
MOTA	143	NHl	ARG	1477	-15.002	1.794	27.549	1.00	33.92
ATOM	146	NH2	ARG	1477	-14.950	4.025	28.062	1.00	31.74
ATOM	149	С	ARG	1477	-10.452	4.266	25.153	1.00	33.13
ATOM	150	0	ARG	1477	-9.777	3.281	25.445	1.00	33.55
ATOM	151	N	LEU	1478	-9.923	5.466	24.984	1.00	34.43
MOTA	153	CA	LEU	1478	-8.493	5.663	25.076	1.00	35.68
ATOM	154	CB	LEU	1478	-8.008	6.350	23.790	1.00	34.98
ATOM	155	CG	LEU	1478	-6.581	6.137	23.284	1.00	31.11
MOTA	156	CD1	LEU	1478	-6.280	4.650	23.161	1.00	26.62
ATOM	157	CD2	LEU	1478	-6.428	6.839	21.940	1.00	28.80
MOTA	158	С	LEU	1478	-8.158	6.505	26.295	1.00	36.21
ATOM	159	0	LEU	1478	-8.501	7.688	26.361	1.00	39.67
ATOM	160	N	VAL	1479	-7.558	5.878	27.293	1.00	35.42
ATOM	162	CA	VAL	1479	-7.156	6.599	28.491	1.00	35.80
ATOM	163	СВ	VAL	1479	-7.269	5.707	29.742	1.00	36.29
MOTA	164	CG1	VAL	1479	-7.017	6.527	30.983	1.00	37.23
ATOM	165	CG2	VAL	1479	-8.650	5.059	29.812	1.00	34.41
ATOM	166	С	VAL	1479	-5.704	7.046	28.244	1.00	35.68
ATOM	167	0	VAL	1479	-4.764	6.246	28.319	1.00	33.45
ATOM	168	N	LEU	1480	-5.538	8.315	27.885	1.00	38.15
MOTA	170	CA	LEU	1480	-4.213	8.860	27.584	1.00	42.61
ATOM	171	СВ	LEU	1480	-4.332	10.205	26.857	1.00	39.14
ATOM	172	CG	LEU	1480	-4.969	10.179	25.460	1.00	38.44
MOTA	173	CD1	TE O	1480	-4.901	11.579	24.879	1.00	39.39
ATOM	174	CD2	LEU	1480	-4.263	9.194	24.533	1.00	36.86
ATOM	175	C	TRA	1480	-3.274	8.970	28.783	1.00	46.37
ATOM	176	0	LEU	1480	~3.659	9.445	29.850	1.00	48.86
MOTA	177	N	GLY	1481	-2.033	8.537	28.594	1.00	47.13
MOTA	179	CA	GLY	1481	-1.081	8.573	29.678	1.00	48.19
MOTA	180	Ċ	GLY	1481	0.163	9.388	29.425	1.00	50.27
MOTA	181	Ö	GLY	1481	0.152	10.367	28.675	1.00	51.19
ATOM	182	N	LYS	1482	1.240	8.965	30.078	1.00	50.93
ATOM	184	CA	LYS	1482	2.543	9.606	30.007	1.00	50.94
ATOM	185	СВ	LYS	1482	3.509	8.866	30.933	1.00	50.41
ATOM	186	CG	LYS	1482	4.971	9.026	30.567	1.00	51.87
ATOM	187	CD	LYS	1482	5.810	7.874	31.087	1.00	53.49
MOTA	188	CE	LYS	1482	5.390	6.542	30.478	1.00	50.77
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ATOM	189	NZ	LYS	1482	6.251	5.433	30.986	1.00	49.92
ATOM	193	C	LYS	1482	3.145	9.676	28.609	1.00	52.31
MOTA	194	0	LYS	1482	3.115	8.700	27.851	1.00	52.30
MOTA	195	N	PRO	1483	3.706	10.838	28.250	1.00	53.47
ATOM	196	CD	PRO	1483	3.667	12.105	28.997	1.00	54.19
ATOM	197	CA	PRO	1483	4.326	11.021	26.937	1.00	54.10
ATOM	198	CB	PRO	1483	4.772	12.480	26.976	1.00	54.25
MOTA	199	CG	PRO	1483	3.772	13.118	27.895	1.00	55.30
ATOM	200	С	PRO	1483	5.535	10.096	26.827	1.00	54.72
ATOM	201	0	PRO	1483	6.343	10.017	27.751	1.00	53.48
ATOM	202	N	LEU	1484	5.619	9.351	25.731	1.00	57.05
MOTA	204	CA	LEU	1484	6.739	8.447	25.503	1.00	59.26
ATOM	205	CB	LEU	1484	6.307	7.241	24.669	1.00	59.35
MOTA	206	CG	LEU	1484	5.391	6.216	25.343	1.00	60.87
ATOM	207	CD1	LEU	1484	4.975	5.161	24.329	1.00	57.14
ATOM	208	CD2	LEU	1484	6.081	5.571	26.551	1.00	59.79
MOTA	209	С	LEU	1484	7.847	9.194	24.778	1.00	61.30
MOTA	210	0	LEU	1484	8.980	8.720	24.701	1.00	62.17
ATOM	211	N	GLY	1485	7.494	10.351	24.220	1.00	63.75
ATOM	213	CA	GLY	1485	8.456	11.173	23.507	1.00	66.33
ATOM	214	C .	GLY	1485	8.081	11.412	22.054	1.00	67.79
ATOM	215	0	GLY	1485	6.918	11.653	21.727	1.00	69.61
ATOM ATOM	216 218	N	GLN	1491	4.615	13.762	18.385	1.00	58.26
ATOM	219	CA CB	GLN GLN	1491	4.353	13.353	19.762	1.00	57.98
ATOM	220	CG	GLN	1491	3.476	14.379	20.468	1.00	61.80
ATOM	221	CD	GLN	1491	3.134	14.034	21.920	1.00	70.31
ATOM	222	OE1	GLN	1491	2.019	14.911	22.482	1.00	75.91
ATOM	223	NE2	GLN	1491 1491	1.355	15.636	21.748	1.00	77.85
ATOM	226	C	GLN	1491	1.820 3.709	14.832	23.788	1.00	78.30
ATOM	227	ō	GLN	1491	2.701	11.965 11.669	19.881	1.00	54.67
ATOM	228	N	VAL	1492	4.305	11.125	19.222	1.00	54.91
MOTA	230	CA	VAL	1492	3.825	9.763	20.729 20.988	1.00	50.04
MOTA	231	СВ	VAL	1492	4.861	8.705	20.583	1.00 1.00	44.93
MOTA	232	CG1	VAL	1492	4.378	7.325	20.958	1.00	42.65 39.71
ATOM	233	CG2	VAL	1492	5.119	8.766	19.099	1.00	40.98
MOTA	234	С	VAL	1492	3.584	9.661	22.490	1.00	43.43
MOTA	235	0	VAL	1492	4.451	10.029	23.289	1.00	43.43
MOTA	236	N	VAL	1493	2.400	9.212	22.888	1.00	41.13
MOTA	238	CA	VAL	1493	2.107	9.080	24.304	1.00	38.77
MOTA	239	CB	VAL	1493	1.052	10.133	24.782	1.00	36.35
MOTA	240	CG1	VAL	1493	1.410	11.508	24.287	1.00	36.06
ATOM	241	CG2	VAL	1493	-0.329	9.755	24.339	1.00	37.64
ATOM	242	С	VAL	1493	1.589	7.693	24.619	1.00	37.77
ATOM	243	0	VAL	1493	0.948	7.058	23.783	1.00	38.88
MOTA	244	N	LEU	1494	1.949	7.187	25.790	1.00	36.24
MOTA	246	CA	LEU	1494	1.468	5.880	26.205	1.00	35.92
MOTA	247	CB	LEU	1494	2.252	5.383	27.429	1.00	35.41
ATOM	248	CG	LEU	1494	1.886	4.009	28.004	1.00	36.21
MOTA	249	CD1	LEU	1494	1.927	2.931	26.924	1.00	33.60
MOTA	250	CD2	LEU	1494	2.835	3.670	29.145	1.00	36.03
ATOM	251	C	LEU	1494	-0.010	6.095	26.564	1.00	35.27
MOTA	252	0	LEU	1494	-0.425	7.215	26.887	1.00	34.35
MOTA	253	N	ALA	1495	-0.807	5.043	26.468	1.00	34.93

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ATOM	255	CA	ALA	1495	-2.220	5.145	26.768	1.00	34.44
ATOM	256	СВ	ALA	1495	-2.955	5.794	25.616	1.00	35.29
ATOM	257	С	ALA	1495	-2.781	3.770	27.018	1.00	34.59
ATOM	258	0	ALA	1495	-2.128	2.766	26.748	1.00	35.52
MOTA	259	N	GLU	1496	-3.996	3.723	27.536	1.00	36.64
ATOM	261	CA	GLU	1496	-4.652	2.462	27.806	1.00	37.57
MOTA	262	СВ	GLU	1496	-5.000	2.354	29.287	1.00	38.97
MOTA	263	CG	GLU	1496	-3.769	2.304	30.185	1.00	41.79
MOTA	264	CD	GLU	1496	-4.110	2.475	31.645	1.00	43.65
MOTA	265	OE1	GLU	1496	-4.408	3.617	32.036	1.00	42.97
ATOM	266	OE2	GLU	1496	-4.086	1.475	32.398	1.00	46.65
ATOM	267	C	GLU	1496	-5.896	2.404	26.943	1.00	38.50
MOTA	268	O	GLU	1496	-6.660	3.371	26.867	1.00	40.28
MOTA	269	N	ALA	1497	-6.051	1.301	26.223	1.00	37.34
MOTA	271	CA	ALA	1497	-7.194	1.131	25.352	1.00	37.42
MOTA	272	CB	ALA	1497	-6.743	0.625	23.985	1.00	35.92
ATOM	273	C	ALA	1497	-8.146	0.148	26.000	1.00	36.77
ATOM	274	0	ALA	1497	-7.759	-0.977	26.323	1.00	35.74
ATOM	275	N	ILE	1498	-9.354	0.616	26.291	1.00	37.03
ATOM	277	CA	ILE	1498	-10.378	-0.224	26.896	1.00	36.80
ATOM	278	CB	ILE	1498	-11.372	0.612	27.728	1.00	34.53
ATOM	279	CG2	ILE	1498	-12.373	-0.290	28.425	1.00	34.59
ATOM	280	CG1	ILE	1498	-10.640	1.438	28.778	1.00	31.97
ATOM	281	CD1	ILE	1498	-11.552	2.344	29.541	1.00	31.12
ATOM	282	С	ILE	1498	-11.126	-0.807	25.709	1.00	38.72
ATOM	283	0	ILE	1498	-11.647	-0.066	24.879	1.00	37.74
ATOM	284	N	GLY	1499	-11.137	-2.126	25.590	1.00	40.98
ATOM	286	CA	GLY	1499	-11.839	-2.728	24.482	1.00	44.64
ATOM	287	С	GLY	1499	-10.931	-3.115	23.332	1.00	48.45
ATOM	288	0	GLY	1499	-10.260	-4.147	23.401	1.00	51.92
ATOM	289	N	LEU	1500	-10.877	-2.269	22.303	1.00	47.87
ATOM	291	CA	LEU	1500	-10.076	-2.530	21.102	1.00	46.80
MOTA	292	CB	LEU	1500	-8.594	-2.770	21.434	1.00	45.37
ATOM	293	CG	LEU	1500	-7.543	-1.661	21.293	1.00	44.84
ATOM	294	CD1	LEU	1500	7-6.174	-2.290	21.450	1.00	43.33
ATOM	295	CD2	LEU	1500	-7.623	-0.959	19.948	1.00	40.43
ATOM	296	C	LEU	1500	-10.631	-3.737	20.349	1.00	45.63
ATOM ATOM	297 298	O N	LEU PRO	1500	-10.797	-4.823	20.915	1.00	44.42 52.13
ATOM	298 299	CD	PRO	1505	-13.569	-5.910 -7.170	25.549	1.00	54.09
ATOM	300	CA	PRO	1505 1505	-14.316 -14.451	-7.170 -4.828	25.398 25.999	1.00	50.46
ATOM	301	CB	PRO	1505	-15.841	-5.455	25.891	1.00	49.86
ATOM	302	CG	PRO	1505	-15.586	-6.898	26.193	1.00	52.17
ATOM	303	C	PRO	1505		-4.370		1.00	
ATOM	304	0	PRO	1505	-14.136 -14.148	-3.180	27.422	1.00	47.75 47.93
ATOM	305		ASN		-14.148		27.710		
ATOM	303	N		1506 1506		-5.313	28.285	1.00	46.20
ATOM	307	CA CB	asn Asn	1506	-13.458 -14.310	-4.986 -5.829	29.666 30.612	1.00	49.52 52.42
ATOM	309	CG	ASN	1506	-14.310	-5.829 -5.489	30.526	1.00	54.50
ATOM	310	OD1	ASN	1506	-16.179	-4.331	30.520	1.00	57.16
ATOM	311	ND2	ASN	1506	-16.179	-4.331 -6.489	30.880	1.00	56.82
ATOM	314	C	ASN	1506	-10.010	-5.124	30.244	1.00	50.65
MOTA	315	0	ASN	1506	-11.573	-5.174	31.178	1.00	50.65
ATOM	316	N	ARG	1507	-11.142	-5.145	28.968	1.00	50.85
AT OF	270	7A	ALCO	TOU/		-3.143	20.700	1.00	JU. JU

ATOM	318	CA	ARG	1507	-9.700	-5.276	29.127	1.00	49.77
MOTA	319	CB	ARG	1507	-9.192	-6.483	28.339	1.00	55.81
MOTA	320	CG	ARG	1507	-9.450	-7.833	28.988	1.00	61.63
ATOM	321	CD	ARG	1507	-8.408	-8.149	30.041	1.00	66.01
MOTA	322	NE	ARG	1507	-8.600	-9.490	30.583	1.00	72.55
ATOM	324	CZ	ARG	1507	-8.024	-9.944	31.694	1.00	77.32
ATOM	325	NHl	ARG	1507	-7.198	-9.169	32.392	1.00	78.41
MOTA	328	NH2	ARG	1507	-8.335	-11.151	32.147	1.00	79.30
ATOM	331	С	ARG	1507	-9.015	-4.036	28.595	1.00	45.60
MOTA	332	0	ARG	1507	-9.452	-3.464	27.590	1.00	42.08
MOTA	333	N	VAL	1508	-7.977	-3.597	29.297	1.00	42.86
MOTA	335	CA	VAL	1508	-7.216	-2.443	28.858	1.00	40.75
MOTA	336	CB	VAL	1508	-6.903	-1.428	30.010	1.00	38.75
MOTA	· 337	CG1	VAL	.1508	8.184	-1.015	30.702	1.00	43.29
MOTA	338	CG2	VAL	1508	-5.919	-2.005	31.012	1.00	37.56
ATOM	339	C	VAL	1508	-5.929	-2.970	28.248	1.00	39.14
MOTA	340	0	VAL	1508	-5.369	-3.972	28.708	1.00	39.16
ATOM	341	N	THR	1509	-5. 51 7	-2.345	27.157	1.00	37.26
MOTA	343	CA	THR	1509	-4.298	-2.737	26.486	1.00	36.52
ATOM	344	CB	THR	1509	-4.571	-3.187	25.019	1.00	37.83
MOTA	345	OG1	THR	1509	-5.423	-4.340	25.011	1.00	43.88
MOTA	347	CG2	THR	1509	-3.267	-3.540	24.310	1.00	34.51
MOTA	348	C	THR	1509	-3.434	-1.495	26.473	1.00	35.82
ATOM	349	0	THR	1509	-3.927	-0.408	26.174	1.00	34.37
ATOM	350	N	LYS	1510	-2.175	-1.628	26.880	1.00	35.96
ATOM	352	CA	LYS	1510	-1.291	-0.479	26.843	1.00	36.13
ATOM	353	CB	LYS	1510	-0.032	-0.695	27.680	1.00	37.77
ATOM	354	CG	LYS	1510	-0.277	-0.854	29.162	1.00	44.58
MOTA	355	CD	LYS	1510	1.023	-0.658	29.948	1.00	51.33
MOTA	356	CE	LYS	1510	0.947	-1.286	31.342	1.00	58.15
ATOM	357	NZ	LYS	1510	-0.149	-0.728	32.187	1.00	64.94
ATOM	361	С	LYS	1510	~0.929	-0.355	25.373	1.00	34.59
ATOM	362	0	LYS	1510	-0.574	-1.345	24.734	1.00	31.43
ATOM	363	N	VAL	1511	-1.092	0.846	24.835	1.00	32.95
ATOM	365	CA	VAL	1511	-0.810	1.121	23.441	1.00	32.29
ATOM	366	CB	VAL	1511	-2.129	1.213	22.621	1.00	32.95
ATOM	367	CG1	VAL	1511	-2.879	-0.109	22.686	1.00	34.79
ATOM	368	CG2	VAL	1511	-3.026	2.354	23.148	1.00	32.84
ATOM	369	C	VAL	1511	-0.058	2.446	23.353	1.00	32.65
ATOM ATOM	370	0	VAL	1511	0.021	3.185	24.344	1.00	31.62
	371	N	ALA	1512	0.521	2.721	22.186	1.00	30.24
ATOM	373	CA	ALA	1512	1.244	3.969	21.954	1.00	28.18
ATOM	374	CB	ALA	1512	2.599	3.700	21.316	1.00	25.62
MOTA MOTA	375	C	ALA	1512	0.373	4.783	21.015	1.00	27.54
	376	0	ALA	1512	-0.151	4.264	20.040	1.00	27.17
ATOM	377	N	VAL	1513	0.204	6.054	21.322	1.00	30.52
MOTA	379	CA	VAL	1513	-0.630	6.914	20.503	1.00	34.08
MOTA	380	CB	VAL	1513	-1.731	7.591	21.347	1.00	34.61
ATOM	381	CG1	VAL	1513	-2.607	8.444	20.474	1.00	36.75
MOTA	382	CG2	VAL	1513	-2.567	6.549	22.087	1.00	33.45
ATOM	383	C	VAL	1513	0.203	8.008	19.837	1.00	36.38
MOTA	384	0	VAL	1513	0.924	8.750	20.510	1.00	35.32
MOTA	385	N	LYS	1514	0.105	8.093	18.513	1.00	38.19
ATOM	387	CA	LYS	1514	0.818	9.104	17.746	1.00	40.12

ATOM	388	CB	LYS	1514	1.339	8.513	16.439	1.00	40.93
ATOM	389	CG	LYS	1514	2.452	7.488	16.632	1.00	42.52
ATOM	390	CD	LYS	1514	2.861	6.803	15.338	1.00	46.25
ATOM	391	CE	LYS	1514	3.268	7.796	14.261	1.00	49.76
ATOM	392	NZ	LYS	1514	4.304	8.771	14.705	1.00	52.14
ATOM	396	С	LYS	1514	-0.166	10.215	17.458	1.00	40.69
ATOM	397	0	LYS	1514	-1.313	9.953	17.110	1.00	41.69
ATOM	398	N	MET	1515	0.277	11.454	17.613	1.00	43.28
ATOM	400	CA	MET	1515	-0.569	12.610	17.379	1.00	46.21
MOTA	401	CB	MET	1515	-1.363	12.936	18.644	1.00	46.96
ATOM	402	CG	MET	1515	-0.488	13.293	19.837	1.00	47.61
ATOM	403	SD	MET	1515	-1.413	13.464	21.358	1.00	49.77
ATOM	404	CE	MET	1515	-1.593	11.761	21.814	1.00	47.84
MOTA	405	С	MET	1515	0.299	13.805	17.000	1.00	49.90
ATOM	406	0	MET	1515	1.519	13.788	17.194	1.00	49.83
MOTA	407	N	LEU	1516	-0.339	14.822	16.430	1.00	54.45
ATOM	409	CA	LEU	1516	0.335	16.053	16.023	1.00	57.57
ATOM	410	CB	LEU	1516	-0.483	16.762	14.944	1.00	54.10
ATOM	411	CG	LEU	1516	-0.800	16.007	13.664	1.00	50.71
ATOM	412	CD1	LEU	1516	-1.830	16.800	12.901	1.00	51.20
ATOM	413	CD2	LEU	1516	0.467	15.809	12.849	1.00	50.08
ATOM	414	C	LEU	1516	0.487	17.010	17.202	1.00	61.88
ATOM	415	0	LEU	1516	-0.170	16.852	18.235	1.00	63.30
ATOM	416	N	LYS	1517	1.335	18.018	17.021	1.00	66.83
ATOM	418	CA	LYS	1517	1.568	19.036	18.037	1.00	71.46
MOTA	419	CB	LYS	1517	2.985	19.593	17.911	1.00	76.28
ATOM	420	CG	LYS	1517	4.084	18.626	18.349	1.00	82.19
MOTA	421	CD	LYS	1517	5.450	19.085	17.846	1.00	86.93
ATOM	422	CE	LYS	1517	6.579	18.228	18.411	1.00	90.46
ATOM	423	NZ	LYS	1517	7.896	18.513	17.763	1.00	92.51
MOTA MOTA	427	C	LYS	1517	0.549	20.156	17.837	1.00	72.44
ATOM	428 429	O N	LYS	1517	-0.142	20.198	16.819	1.00	72.12
ATOM	431	CA	SER SER	1518	0.474	21.075	18.793	1.00	73.90
ATOM	432	CB		1518	-0.470	22.185	18.697	1.00	74.96
ATOM	433	C	SER SER	1518	-0.498	22.980	20.002	1.00	74.72
ATOM	434	0		1518	-0.133	23.100	17.525	1.00	76.16
ATOM	435	N	SER ASP	1518 1519	-1.029 1. 1 58	23.667	16.897	1.00	76.56
ATOM	437	CA	ASP	1519	1.601	23.245 24.094	17.232 16.125	1.00 1.00	77.24
ATOM	438	CB	ASP	1519	2.849	24.888	16.535	1.00	78.51 79.70
MOTA	439	C	ASP	1519	1.887	23.264	14.865	1.00	78.29
ATOM	440	ō	ASP	1519	2.797	23.580	14.088	1.00	78.52
ATOM	441	N	ALA	1520	1.121	22.192	14.682	1.00	76.90
ATOM	443	CA	ALA	1520	1.285	21.313	13.529	1.00	74.09
ATOM	444	СВ	ALA	1520	0.737	19.930	13.840	1.00	74.20
ATOM	445	C	ALA	1520	0.580	21.895	12.318	1.00	71.82
ATOM	446	0	ALA	1520	-0.573	22.311	12.400	1.00	71.02
ATOM	447	N	THR	1521	1.291	21.951	11.202	1.00	69.97
ATOM	449	CA	THR	1521	0.734	22.480	9.970	1.00	68.86
ATOM	450	CB	THR	1521	1.848	22.911	9.026	1.00	68.87
ATOM	451	OG1	THR	1521	2.621	21.762	8.651	1.00	70.03
MOTA	453	CG2	THR	1521	2.756	23.912	9.715	1.00	70.03
ATOM	454	C	THR	1521	-0.081	21.389	9.292	1.00	67.89
ATOM	455	0	THR	1521	0.111	20.204	9.563	1.00	
		~	TILL	1041	0.111	20.204	9.303	1.00	69.03

ATOM	456	N	GLU	1522	-0.964	21.783	8.382	1.00	66.59
ATOM	458	CA	GLU	1522	-1.785	20.821	7.657	1.00	65.71
ATOM	459	CB	GLU	1522	-2.737	21.532	6.692	1.00	65.61
MOTA	460	C	GLU	1522	-0.886	19.823	6.909	1.00	64.32
ATOM	461	0	GLU	1522	-1.324	18.729	6.549	1.00	66.29
ATOM	462	N	LYS	1523	0.367	20.205	6.677	1.00	59.93
ATOM	464	CA	LYS	1523	1.314	19.326	6.016	1.00	57.38
ATOM	465	CB	LYS	1523	2.629	20.064	5.747	1.00	60.47
ATOM	466	CG	LYS	1523	3.815	19.162	5.370	1.00	62.75
ATOM	467	CD	LYS	1523	3.510	18.288	4.160	1.00	63.95
ATOM	468	CE	LYS	1523	4.759	17.596	3.652	1.00	65.88
ATOM	469	NZ	LYS	1523	4.429	16.721	2.494	1.00	70.37
ATOM	473	C	LYS	1523	1.565	18.173	6.974	1.00	54.80
ATOM	474	0	LYS	1523	1.548	17.003	6.581	1:00	54.44
ATOM	475	N	ASP	1524	1.786	18.523	8.239	1.00	51.67
ATOM	477	CA	ASP	1524	2.036	17.549	9.295	1.00	49.43
ATOM	478	СВ	ASP	1524	2.297	18.271	10.622	1.00	51.06
ATOM	479	CG	ASP	1524	3.598	19.080	10.622	1.00	54.03
ATOM	480	OD1	ASP	1524	3.649	20.136	11.283	1.00	56.32
ATOM	481	OD2	ASP	1524	4.580	18.658	9.956	1.00	
ATOM	482	C	ASP	1524	0.847	16.596	9.413	1.00	56.02
ATOM	483	ō	ASP	1524	1.017	15.387	9.580	1.00	47.73 45.85
ATOM	484	N	LEU	1525	-0.354	17.155	9.300	1.00	47.62
ATOM	486	CA	LEU	1525	-1.585	16.380	9.354	1.00	45.95
ATOM	487	СВ	LEU	1525	-2.801	17.307	9.271	1.00	43.61
ATOM	488	CG	LEU	1525	-4.193	16.665	9.234	1.00	.44.56
ATOM	489	CD1	LEU	1525	-4.364	15.543	10.268	1.00	46.02
ATOM	490	CD2	LEU	1525	-5.215	17.740	9.468	1.00	43.80
ATOM	491	С	LEU	1525	-1.605	15.372	8.210	1.00	45.67
MOTA	492	0	LEU	1525	-1.921	14.204	8.416	1.00	46.78
ATOM	493	N	SER	1526	-1.245	15.822	7.014	1.00	45.44
MOTA	495	CA	SER	1526	-1.211	14.945	5.851	1.00	46.33
MOTA	496	CB	SER	1526	-0.903	15.744	4.584	1.00	48.48
MOTA	497	OG	SER	1526	-2.012	16.546	4.218	1.00	57.28
MOTA	499	C	SER	1526	-0.192	13.821	5.995	1.00	43.84
ATOM	500	0	SER	1526	-0.480	12.669	5.674	1.00	45.24
MOTA	501	N	ASP	1527	0.994	14.144	6.489	1.00	40.88
MOTA	503	CA	ASP	1527	2.024	13.128	6.646	1.00	39.70
MOTA	504	CB	ASP	1527	3.376	13.767	6.960	1.00	37.62
MOTA	505	CG	ASP	1527	3.934	14.555	5.786	1.00	37.01
ATOM	506	OD1	ASP	1527	3.399	14.434	4.657	1.00	35.78
MOTA	507	OD2	ASP	1527	4.916	15.295	5.992	1.00	40.23
MOTA	508	C	ASP	1527	1.652	12.053	7.659	1.00	38.51
ATOM	509	0	ASP	1527	1.951	10.872	7.461	1.00	37.68
MOTA	510	N	LEU	1528	0.973	12.460	8.725	1.00	38.16
MOTA	512	CA	LEU	1528	0.532	11.513	9.744	1.00	38.29
MOTA	513	CB	LEU	1528	0.026	12.258	10.985	1.00	37.12
ATOM	514	CG	LEU	1528	-0.505	11.412	12.153	1.00	39.03
ATOM	515	CD1	LEU	1528	0.499	10.323	12.539	1.00	35.39
MOTA	516	CD2	LEU	1528	-0.825	12.315	13.334	1.00	35.29
ATOM	517	С	LEU	1528	-0.568	10.611	9.155	1.00	38.10
ATOM	518	0	LEU	1528	-0.607	9.400	9.413	1.00	37.21
ATOM	519	N	ILE	1529	-1.450	11.210	8.355	1.00	36.71
ATOM	521	CA	ILE	1529	-2.531	10.472	7.718	1.00	35.93

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MOTA 522 CB ILE 1529 -3.486 11.419 6.931 1.00 35.67 MOTA 523 CG₂ ILE 1529 -4.492 10.619 6.119 1.00 34.04 MOTA 524 CG1 ILE 1529 -4.259 12.295 7.916 1.00 33.81 **ATOM** 525 CD1 ILE 1529 -5.177 13.288 7.276 1.00 33.58 526 MOTA C ILE 1529 -1.912 9.447 6.786 1.00 37.49 **ATOM** 527 O ILE 1529 -2.274 8.269 6.829 1.00 37.11 MOTA 528 N SER 1530 -0.926 9.893 6.003 1.00 38.20 MOTA 530 CA SER 1530 -0.217 9.036 5.050 1.00 37.49 ATOM 531 CB SER 1530 0.911 9.822 4.370 1.00 43.32 **ATOM** 532 OG SER 1530 0.424 10.970 3.687 1.00 52.31 **MOTA** 534 ¢ SER 1530 0.382 7.808 5.719 1.00 34.40 MOTA 535 SER 0 1530 0.234 6.691 1.00 5.219 31.51 **ATOM** 536 N GLU 1531 1.048 8.028 6.851 1.00 32.08 MOTA 53B GLU CA 1531 1.690 6.952 7.594 1.00 30.60 ATOM " 539 CB GLU 1531 2.506 7.515 8.759 1.00 29.70 **ATOM** 540 CG GLU 1531 3.094 9.657 6.428 1.00 30.53 **MOTA** 541 CD GLU 1531 3.871 6.962 10.839 1.00 33.17 MOTA 542 OE1 GLU 1531 4.473 6.134 11.552 1.00 33.38 MOTA 543 OE2 GLU 1531 3.883 8.193 11.062 1.00 37.52 ATOM 544 C GLU 1531 0.698 5.911 **B.094** 1.00 30.17 **ATOM** 545 0 GLU 1531 0.991 4.714 8.100 1.00 29.76 ATOM 546 N MET 1532 -0.464 6.379 8.530 1.00 31.34 **ATOM** 548 CA MET 1532 -1.521 5.496 9.015 1.00 30.72 ATOM 549 CB MET 1532 -2.666 6.336 9.591 1.00 29.99 ATOM 550 CG MET 1532 -3.880 5.523 10.020 1.00 30.10 MOTA 551 SD MET 1532 -5.173 6.510 10.727 1.00 29.46 MOTA 552 CE MET 1532 -5.462 7.682 9.455 1.00 23.76 **ATOM** 553 1532 C MET -2.025 4.638 7.843 1.00 30.47 **ATOM** 554 o MET 1532 -2.080 3.401 7.925 1.00 27.05 **ATOM** 555 N GLU 1533 -2.387 5.319 6.756 1.00 30.56 ATOM 557 CA GLU 1533 -2.863 4.674 5.542 1.00 30.56 ATOM 558 CB GLU 1533 -3.090 5.725 4.458 1.00 28.60 MOTA 559 CG GLU 1533 -4.226 6.677 4.761 1.00 29.08 MOTA 560 CD GLU 1533 -5.531 5.954 5.014 1.00 31.28 **MOTA** 561 OE1 GLU 1533 -6.006 5.230 4.117 1.00 33.09 ATOM 562 OE2 GLU 1533 -6.086 6.104 6.121 1.00 34.97 MOTA 563 C GLU -1.861 1533 3.638 5.064 1.00 29.86 **ATOM** 564 0 GLU 1533 -2.232 2.541 4.677 1.00 32.28 ATOM 565 N MET 1534 -0.590 4.014 5.107 1.00 32.54 MOTA 567 CA MET 1534 0.515 3.145 4.719 1.00 33.39 MOTA 568 CB MET 1534 1.826 3.894 4.885 1.00 34.70 MOTA 569 CG MET 1534 3.038 3.047 44.51 4.654 1.00 MOTA 570 SD MET 1534 3.479 3.063 2.943 1.00 52.81 MOTA 571 CE MET 1534 4.349 4.607 2.874 1.00 47.34 MOTA 572 С MET 1534 0.530 1.896 5.607 1.00 32.98 MOTA 573 0 MET 1534 0.689 0.776 5.115 1.00 34.00 MOTA 574 N MET 1535 0.364 2.100 6.910 1.00 31.92 MOTA 576 CA MET 1535 0.336 0.986 7.848 1.00 30.80 ATOM 577 CB MET 1535 0.252 1.503 33.77 9.294 1.00 **ATOM** 578 CG MET 1535 1.509 2.216 9.810 1.00 32.26 MOTA 579 SD MET 1535 1.520 2.433 11.617 1.00 34.75 ATOM 580 CE MET 1535 1.183 4.173 11.723 1.00 37.86 **ATOM** 581 C MET 1535 -0.837 0.052 7.521 1.00 30.80 MOTA 582 O MET 1535 -0.704 -1.175 7.589 1.00 32.03

MOTA	583	N	LYS	1536	-1.974	0.638	7.142	1.00	31.04		
MOTA	585	CA	LYS	1536	-3.170	-0.123	6.767	1.00	31.15		
ATOM	586	CB	LYS	1536	-4.334	0.808	6.415	1.00	31.21	•	
ATOM	587	CG	LYS	1536	-4.864	1.625	7.552	1.00	27.76		
ATOM	588	CD	LYS	1536	-5.973	2.540	7.103	1.00	21.44		
ATOM	589	CE	LYS	1536	-6.434	3.401	8.248	1.00	24.69	-	
ATOM	590	NZ	LYS	1536	-7.578	4.241	7.868	1.00	25.84		
MOTA	594	С	LYS	1536	-2.887	-1.003	5.561	1.00	30.71		
ATOM	595	0	LYS	1536	-3.238	-2.175	5.560	1.00	34.73		
ATOM	596	N	MET	1537	-2.309	-0.412	4.523	1.00	31.18	•	
ATOM	598	CA	MET	1537	-1.967	-1.148	3.307	1.00	31.53		
MOTA	599	CB	MET	1537	-1.370	-0.200	2.267	1.00	35.11		
MOTA	600	CG	MET	1537	-2.377	0.780	1.654	1.00	42.40		
ATOM	601	SD	MET -	1537	-3.657	-0.051	0.685	1.00	50:10	 	
ATOM	602	CE	MET	1537	-3.069	0.266	-0.972	1.00	50.20		
ATOM	603	C	MET	1537	-0.976	-2.276	3.572	1.00	30.86		
ATOM	604	0	MET	1537	-1.218	-3.425	3.210	1.00	30.07		
ATOM	605	N	ILE	1538	0.119	-1.950	4.259	1.00	30.92		
ATOM	607	CA	ILE	1538	1.173	-2.923	4.563	1.00	28.12		
ATOM	608	CB	ILE	1538	2.359	-2.254	5.313	1.00	28.71		
ATOM	609	CG2	ILE	1538	3.310	-3.303	5.865	1.00	29.72		
MOTA	610	CG1	ILE	1538	3.126	-1.343	4.350	1.00	30.79		
ATOM	611	CD1	ILE	1538	4.375	-0.745	4.945	1.00	32.46		
ATOM	612	C	ILE	1538	0.717	-4.179	5.299	1.00	26.33		
ATOM	613	0	ILE	1538	1.178	-5.276	4.996	1.00	24.20		
MOTA	614	N	GLY	1539	-0.188	-4.027	6.258	1.00	27.41		
ATOM	616	CA	GLY	1539	-0.651	-5.190	6.997	1.00	27.83		
MOTA	617	C	GLY	1539	0.240	-5.533	8.179	1.00	29.10		
MOTA	618	0	GLY	1539	1.308	-4.937	8.368	1.00	30.33		
MOTA	619	N	LYS	1540	-0.157	-6.561	8.916	1.00	29.46		
MOTA	621	CA	LYS	1540	0.539	-6.976	10.120	1.00	29.27		
MOTA	622	CB	LYS	1540	-0.470	-7.520	11.139	1.00	27.01		
MOTA	623	CG	LYS	1540	-1.438	-6.483	11.638	1.00	29.58		
ATOM	624	CD	LYS	1540	-2.496	-7.103	12.530	1.00	39.41		
ATOM	625	CE	LYS	1540	-3.548	-6.069	12.952	1.00	44.14		
ATOM	626	NZ	LYS	1540	-2.994	-4.996	13.828	1.00	46.92		
ATOM	630	С	LYS	1540	1.679	-7.962	10.020	1.00	27.17		
ATOM	631	0	LYS	1540	1.745	-8.794	9.111	1.00	26.20		
MOTA	632	N	HIS	1541	2.565	-7.856	11.006	1.00	26.96		
ATOM	634	CA	HIS	1541	3.690	-8.761	11.144	1.00	27.30		
MOTA	635	CB	HIS	1541	4.787	-8.506	10.120	1.00	22.20		
ATOM	636	CG	HIS	1541	5.849	-9.555	10.125	1.00	21.32		
ATOM	637	CD2	HIS	1541	5.886	-10.789	9.555	1.00	23.29		
ATOM	638	ND1	HIS	1541	7.052	-9.413	10.791	1.00	19.41		
MOTA	640	CE1	HIS	1541	7.775	-10.509	10.633	1.00	23.61		
ATOM	641	NE2	HIS	1541	7.097	-11.355	9.889	1.00	21.81		
MOTA	643	С	HIS	1541	4.245	-8.640	12.565	1.00	28.64		
ATOM	644	0	HIS	1541	4.290	-7.549	13.132	1.00	30.64		
ATOM	645	N	LYS	1542	4.650	-9.791	13.108	1.00	29.47		
ATOM	647	CA	LYS	1542	5.200	-9.893	14.457	1.00	28.78		
MOTA	648	CB	LYS	1542	5.683	-11.326	14.714	1.00	30.16		
ATOM	649	CG	LYS	1542	6.232	-11.572	16.112	1.00	32.63		
MOTA	650	CD	LYS	1542	5.277	-11.046	17.155	1.00	42.90		
MOTA	651	CE	LYS	1542	5.659	-11.475	18.551	1.00	48.13		

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ATOM LYS 1542 4.726 -10.930 19.564 1.00 54.87 652 NZ ATOM C LYS 1542 6.351 -8.928 14.705 1.00 26.54 656 1.00 MOTA 657 0 LYS 1542 6.440 -8.321 15.773 26.19 MOTA 65B ASN 1543 7.193 -8.733 13.697 1.00 24.36 N MOTA 660 CA ASN 1543 8.357 -7.874 13.852 1.00 24.08 ATOM 661 CB **ASN** 1543 9.601 -8.596 13.359 1.00 22.69 MOTA 662 CG **ASN** 1543 9.781 -9.950 14.029 1.00 22.81 ATOM 663 OD1 ASN 1543 9.664 -10.996 13.388 1.00 23.62 MOTA 664 ND2 ASN 1543 10.028 -9.938 15.324 1.00 24.94 MOTA 667 C ASN 1543 8.318 -6.429 13.377 1.00 23.48 ATOM 668 0 ASN 1543 9.351 -5.861 13.059 1.00 22.94 MOTA 669 N ILE 1544 7.130 -5.821 13.380 1.00 24.15 671 MOTA CA ILE 13.012 1544 6.976 -4.407 1.00 24.60 ATOM 672 CB ILE -4.191 1544 6.516 11.531 1.00 24.90 ATOM 673 CG2 ILE 1544 7.495 -4.852 10.571 1.00 21.57 MOTA 674 CG1 ILE 1544 5.081 -4.688 11.316 1.00 26.66 MOTA 675 CD1 ILE 4.481 1544 -4.321 9.945 1.00 23.98 **ATOM** 676 C ILE 1544 5.954 -3.785 13.955 1.00 24.78 MOTA 677 ILE 5.160 O 1544 -4.503 14.558 1.00 27.87 MOTA 678 N ILE 1545 6.035 -2.474 14.159 1.00 26.39 MOTA 680 ILE 5.089 CA 1545 -1.779 15.025 1.00 26.79 MOTA 681 CB ILE 5.588 1545 -0.345 15.384 1.00 28.85 ATOM 682 CG2 ILE 1545 4.512 0.449 16.103 1.00 23.60 MOTA 683 CG1 ILE 1545 6.833 -0.423 16.269 1.00 27.20 MOTA 684 CD1 ILE 1545 6.565 -0.990 17.639 1.00 27.12 MOTA 685 С ILE 1545 3.792 -1.708 1.00 14.224 26.99 MOTA 1545 686 ILE 3.720 O -1.023 13.197 1.00 27.61 ATOM 687 ASN 1546 N 2.809 -2.495 14.654 1.00 26.70 ATOM 689 1546 CA ASN 1.514 -2.565 13.983 1.00 26.53 ATOM 690 CB **ASN** 1546 0.871 -3.953 14.169 1.00 26.23 ATOM 691 CG ASN 1546 1.695 -5.072 13.551 1.00 24.96 MOTA 692 ASN 1546 1.773 OD1 -5.206 12.330 1.00 28.08 MOTA 693 ND2 ASN 1546 2.319 -5.872 14.387 1.00 22.38 **ATOM** 696 C ASN 1546 0.521 -1.497 14.418 1.00 26.89 **ATOM** 697 0 ASN 1546 0.610 -0.952 15.523 1.00 27.40 MOTA 698 N LEU 1547 -0.349 -1.138 13.481 1.00 27.77 MOTA 700 CA LEU 1547 -1.416 -0.175 13.701 1.00 28.28 **ATOM** 701 CB LEU 1547 -1.958 0.313 12.361 1.00 27.04 ATOM 702 CG LEU 1547 -3.199 1.194 12.408 1.00 25.74 MOTA 703 LEU CD1 1547 -2.836 2.575 12.950 1.00 27.66 MOTA 11.014 704 CD2 LEU 1547 -3.799 1.289 1.00 23.38 MOTA 705 C LEU 1547 -2.498 -0.972 14.435 1.00 29.80 **ATOM** 706 LEU 0 1547 ~2.766 -2.135 14.105 1.00 28.63 **ATOM** 707 N LEU 1548 -3.088 -0.351 15.448 1.00 29.91 MOTA 709 CA LEU 1548 -4.114 -0.997 16.256 1.00 28.46 **ATOM** 710 CB LEU 1548 -3.735 -0.956 17.749 1.00 26.76 MOTA 711 CG LEU 1548 -2.460 -1.701 18.162 1.00 22.44 MOTA 712 CD1 LEU 1548 -2.277 -1.554 19.653 1.00 21.91 ATOM 713 CD2 LEU 1548 -2.551 -3.179 17.778 1.00 20.79 **ATOM** 714 C LEU 1548 -5.480 -0.365 16.058 1.00 27.31 1.00 **ATOM** 715 0 LEU 1548 -6.489 -1.043 16.193 28.25 MOTA 716 N GLY 1549 -5.506 0.925 15.732 1.00 24.02 MOTA 718 CA GLY 1549 -6.774 1.598 15.553 1.00 24.57 ATOM 719 C GLY 1549 -6.548 3.077 15.395 1.00 25.19

ATOM	720	0	GLY	1549	-5.400	3.488	15.231	1.00	28.77
ATOM	721	N	ALA	1550	-7.617	3.875	15.427	1.00	24.66
ATOM	723	CA	ALA	1550	-7.487	5.319	15.282	1.00	24.17
MOTA	724	CB	ALA	1550	-7.206	5.680	13.824	1.00	24.29
MOTA	725	C	ALA	1550	-8.695	6.103	15.765	1.00	23.95
ATOM	726	0	ALA	1550	-9.810	5.590	15.780	1.00	24.95
MOTA	727	N	CYS	1551	-8.444	7.336	16.199	1.00	25.03
MOTA	729	CA	CYS	1551	-9.482	8.270	16.639	1.00	28.21
ATOM	730	CB	CYS	1551	-9.221	8.774	18.055	1.00	26.76
ATOM	731	SG	CYS	1551	-9.378	7.521	19.317	1.00	34.39
MOTA	732	С	CYS	1551	-9.359	9.426	15.656	1.00	29.98
MOTA	733	0	CYS	1551	-8.482	10.281	15.800	1.00	32.14
ATOM	734	N	THR	1552	-10.198	9.412	14.625	1.00	31.09
ATOM	736	CA	THR	1552	-10.135	10.435	13.595	1:00	32:91
ATOM	737	CB	THR	1552	-10.052	9.781	12.189	1.00	32.60
ATOM	738	OG1	THR	1552	-11.276	9.097	11.890	1.00	32.12
ATOM	740	CG2	THR	1552	-8.928	8.768	12.144	1.00	32.74
ATOM	741	С	THR	1552	-11.282	11.419	13.591	1.00	35.26
ATOM	742	0	THR	1552	-11.171	12.525	13.057	1.00	35.10
ATOM	743	N	GLN	1553	-12.397	11.014	14.179	1.00	39.01
ATOM	745	CA	GLN	1553	-13.585	11.846	14.180	1.00	41.97
MOTA	746	CB	GLN	1553	-14.832	10.968	14.020	1.00	41.17
ATOM	747	CG	GLN	1553	-14.915	10.238	12.672	1.00	39.06
MOTA	748	CD	GLN	1553	-14.900	11.200	11.496	1.00	41.84
ATOM	749	OE1	GLN	1553	-15.785	12.045	11.359	1.00	41.92
MOTA	750	NE2	GLN	1553	-13.876	11.090	10.652	1.00	42.33
MOTA	75 3	C	GLN	1553	-13.727	12.777	15.372	1.00	45.35
MOTA	754	0	GLN	1553	-13.358	12.423	16.489	1.00	47.02
MOTA	75 5	N	ASP	1554	-14.225	13.981	15.090	1.00	48.60
ATOM	757	CA	ASP	1554	-14.479	15.016	16.084	1.00	50.64
ATOM	758	CB	ASP	1554	-15.832	14.766	16.758	1.00	54.52
ATOM	759	CG	ASP	1554	-17.003	14.955	15.809	1.00	60.54
MOTA	760	OD1	ASP	1554	-18.072	15.409	16.274	1.00	66.04
ATOM	761	OD2	ASP	1554	-16.860	14.661	14.601	1.00	65.09
ATOM	762	C	ASP	1554	-13.395	15.173	17.133	1.00	49.89
ATOM	763	0	ASP	1554	-13.611	14.879	18.310	1.00	51.48
ATOM	764	N	GLY	1555	-12.232	15.643	16.699	1.00	48.40
ATOM	766	CA	GLY	1555	-11.131	15.834	17.617	1.00	46.16
ATOM	767	С	GLY	1555	-9.798	15.626	16.935	1.00	44.64
ATOM	768	0	GLY	1555	-9. 7 37	15.581	15.716	1.00	45.22
ATOM	769	N	PRO	1556	-8.708	15.525	17.702	1.00	44.68
ATOM	770	CD	PRO	1556	-8.672	15.683	19.164	1.00	45.39
ATOM	771	CA	PRO	1556	-7.359	15.326	17.177	1.00	42.95
ATOM	772	CB	PRO	1556	-6.484	15.549	18.411	1.00	43.74
MOTA	773	CG	PRO	1556	-7.354	16.347	19.345	1.00	47.32
ATOM	774	С	PRO	1556	-7.164	13.912	16.665	1.00	42.34
ATOM	775	0	PRO	1556	-7.636	12.953	17.287	1.00	42.75
ATOM	7 76	N	LEU	1557	-6.451	13.788	15.547	1.00	39.83
MOTA	778	CA	LEU	1557	-6.169	12.490	14.954	1.00	36.64
ATOM	779	СВ	LEU	1557	-5.496	12.669	13.587	1.00	34.49
MOTA	780	CG	LEU	1557	-5.009	11.404	12.870	1.00	31.29
MOTA	781	CD1	LEU	1557	-6.169	10.436	12.628	1.00	27.86
MOTA	782	CD2	LEU	1557	-4.314	11.775	11.570	1.00	25.40
ATOM	783	С	LEU	1557	-5.244	11.732	15.894	1.00	35.44

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MOTA 784 0 LEU 1557 -4.210 12..264 16.316 1.00 36.12 MOTA 785 N TYR 1558 -5.664 10.539 16.292 1.00 32.49 MOTA 787 CA TYR 1558 -4.861 9.697 17.157 1.00 31.87 **ATOM** 788 CB TYR 1558 -5.590 9.348 18.470 1.00 33.93 ATOM 789 TYR 1558 -5.695 10.476 1.00 35.34 CG 19.471 ATOM 790 CD1 TYR 1558 -6.566 10.394 20.565 1.00 37.12 **ATOM** 791 CE1 TYR 1558 -6.6B3 11.456 21.479 1.00 36.44 ATOM 792 CD2 TYR 1558 -4.945 11.636 19.317 1.00 37.27 ATOM 793 CE2 TYR 1558 -5.054 12.690 20.213 1.00 39.62 MOTA 794 CZTYR -5.921 1558 12.598 21.289 1.00 40.05 **ATOM** 795 OH TYR 1558 -6.008 13.668 22.155 1.00 44.98 **ATOM** 797 C TYR 1558 -4.600 8.419 16.387 1.00 31.58 ATOM 798 0 TYR 1558 -5.532 7.750 15.936 1.00 30.22 ATOM 799 N VAL 1559 -3.331 8.129 16.153 1.00 33.43 ATOM 801 VAL CA 1559 -2.947 15.463 6.907 1.00 31.42 ATOM 802 VAL CB 1559 -1.849 7.160 14.419 1.00 32.31 ATOM VAL 803 CG1 1559 -1.516 5.851 13.675 1.00 26.79 ATOM 804 CG₂ VAL 1559 -2.308 13.453 8.265 1.00 30.63 ATOM 805 VAL 1559 С -2.438 5.979 16.556 1.00 28.67 MOTA 806 0 VAL 1559 -1.393 17.155 1.00 6.223 30.08 ATOM 807 N ILE 1560 -3.230 4.960 16.852 1.00 25.80 MOTA 809 CA ILE 1560 -2.915 3.998 17.894 1.00 25.33 MOTA 810 CB ILE 1560 -4.2193.443 18.506 1.00 22.34 **ATOM** 811 CG2 ILE 1560 -3.931 2.695 19.784 1.00 20.36 **ATOM** 812 CG1 ILE 1560 -5.172 4.603 18.809 1.00 21.34 ATOM 813 CD1 ILE 1560 -6.583 4.190 19.093 1.00 20.68 **ATOM B14** С ILE 1560 -2.073 2.857 1.00 17.341 27.16 **ATOM** 1560 **B15** 0 ILE -2.520 2.116 16.455 1.00 29.67 ATOM 816 N VAL 1561 -0.858 2.714 17.860 1.00 27.69 **ATOM** 818 CA VAL 1561 0.060 1.667 17.411 1.00 28.27 ATOM 819 CB VAL 1561 1.311 2.269 16.696 1.00 27.34 **MOTA** 820 CG1 VAL 1561 0.892 3.019 15.445 1.00 21.76 **ATOM** 821 CG2 VAL 1561 2.074 3.201 17.639 1.00 26.00 **ATOM** 822 C VAL 1561 0.509 0.809 18.588 1.00 28.70 MOTA 823 0 VAL 1561 0.221 1.139 19.746 1.00 30.52 MOTA 824 N GLU 1562 1.166 -0.311 18.286 1.00 28.64 **ATOM** 826 CA GLU 1562 1.658 -1.220 19.318 1.00 27.77 **ATOM** 827 CB GLU 1562 2.278 -2.465 18.693 1.00 24.57 **MOTA** 828 CG GLU 1562 1.251 ~3.452 18.208 1.00 24.76 **ATOM** 829 CD GLU 1562 1.864 -4.641 17.501 1.00 27.27 MOTA 830 OE1 GLU 1562 1.272 -5.739 1.00 17.580 28.27 **ATOM** 831 OE2 GLU 1562 2.920 -4.487 16.849 1.00 29.25 MOTA 832 C GLU 1562 2.674 -0.538 20.217 1.00 28.79 MOTA 833 0 GLU 1562 3.453 0.292 19.760 1.00 29.38 **ATOM** 834 N TYR 1563 2.627 -0.871 21.503 1.00 30.84 MOTA 836 CA TYR 1563 3.534 -0.304 22.493 1.00 31.43 MOTA 837 CB TYR 1563 2.782 -0.088 23.799 1.00 32,10 **ATOM** 838 CG TYR 1563 3.632 0.376 24.952 1.00 33.93 MOTA 839 CD1 TYR 1563 4.366 1.552 24.873 1.00 34.85 **ATOM** 840 CE1 TYR 1563 5.140 1.992 25.947 1.00 37.53 ATOM 841 CD2 TYR 1563 3.683 -0.356 26.136 1.00 34.81 **ATOM** 842 CE2 TYR 1563 4.452 0.072 27.211 1.00 34.01 ATOM 843 CZ1563 TYR 5.173 1.245 27.113 1.00 35.79 ATOM 844 OH 1563 TYR 5.920 1.677 28.184 1.00 39.10

ATOM	846	C	TYR	1563	4.767	-1.166	22.731	1.00	31.38
ATOM	847	0	TYR	1563	4.672	-2.385	22.905	1.00	30.73
ATOM	848	N	ALA	1564	5.930	-0.525	22.725	1.00	32.23
ATOM	850	CA	ALA	1564	7.198	-1.212	22.953	1.00	35.90
ATOM	851	CB	ALA	1564	8.178	-0.866	21.833	1.00	36.44
ATOM	852	C	ALA	1564	7.711	-0.719	24.307	1.00	36.52
MOTA	85 3	0	ALA	1564	8.332	0.349	24.403	1.00	39.16
ATOM	854	N	SER	1565	7.424	-1.482	25.359	1.00	34.62
MOTA	856	CA	SER	1565	7.801	-1.071	26.700	1.00	34.91
MOTA	857	CB	SER	1565	7.124	-1.945	27.750	1.00	32.11
MOTA	858	OG	SER	1565	7.606	-3.271	27.696	1.00	32.92
ATOM	860	С	SER	1565	9.288	-0.968	26.996	1.00	35.56
ATOM	861	0	SER	1565	9.674	-0.219	27.886	1.00	38.69
MOTA	862	N	LYS	1566	10.127	-1.673	26.243	1:00	33:70
MOTA	864	CA	LYS	1566	11.557	-1.625	26.526	1.00	31.40
ATOM	865	CB	LYS	1566	12.137	-3.033	26.530	1.00	30.56
ATOM	866	CG	LYS	1566	11.555	-3.869	27.664	1.00	32.32
MOTA	867	CD	LYS	1566	11.997	-5.308	27.599	1.00	36.47
MOTA	868	CE	LYS	1566	11.632	-6.031	28.872	1.00	36.97
MOTA	869	NZ	LYS	1566	12.104	-7.436	28.804	1.00	41.62
MOTA	873	С	LYS	1566	12.380	-0.664	25.683	1.00	32.18
ATOM	874	0	LYS	1566	13.616	-0.691	25.715	1.00	32.57
ATOM	875	N	GLY	1567	11.686	0.223	24.973	1.00	33.39
ATOM	877	CA	GLY	1567	12.345	1.224	24.156	1.00	32.13
ATOM	878	C	GLY	1567	13.074	0.719	22.928	1.00	31.70
ATOM	879	О	GLY	1567	12.912	-0.430	22.530	1.00	33.30
ATOM	880	N	ASN	1568	13.883	1.589	22.331	1.00	31.08
ATOM	882	CA	ASN	1568	14.632	1.230	21.139	1.00	31.00
MOTA	883	CB	ASN	1568	15.066	2.478	20.365	1.00	31.30
MOTA	884	CG	ASN	1568	16.127	3.271	21.074	1.00	30.47
ATOM	885	OD1	ASN	1568	17.130	2.733	21.508	1.00	32.19
ATOM	886	ND2	ASN	1568	15.934	4.580	21.144	1.00	32.13
ATOM	889	С	ASN	1568	15.802	0.295	21.393	1.00	30.62
ATOM	890	0	ASN	1568	16.357	0.256	22.483	1.00	32.91
ATOM	891	N	LEU	1569	16.193	-0.428	20.354	1.00	30.92
ATOM	893	CA	LEU	1569	17.269	~1.403	20.417	1.00	31.22
ATOM	894	CB	LEU	1569	17.418	-2.083	19.054	1.00	29.57
ATOM	895	CC	LEU	1569	18.415	-3.231	18.893	1.00	29.22
ATOM ATOM	896	CD1	LEU	1569	18.284	-4.261	20.024	1.00	21.30
	897	CD2	LEU	1569	18.184	-3.863	17.523	1.00	24.99
ATOM ATOM	898 899	C	LEU	1569	18.609	-0.838	20.878	1.00	32.44
ATOM		0	LEU	1569	19.328	-1.499	21.618	1.00	33.12
ATOM	900	N	ARG	1570	18.954	0.370	20.432	1.00	33.24
	902	CA	ARG	1570	20.218	0.983	20.834	1.00	33.01
ATOM ATOM	903 904	CB	ARG	1570	20.348	2.394	20.256	1.00	32.36
ATOM		CC	ARG	1570	21.586	3.129	20.758	1.00	38.28
	905	CD	ARG	1570	21.672	4.538	20.221	1.00	41.93
ATOM ATOM	906	NE CZ	ARG	1570	20.428	5.278	20.412	1.00	49.82
ATOM	908	CZ	ARG	1570	19.975	5.721	21.584	1.00	52.37
ATOM	909	NH1	ARG	1570	20.659	5.510	22.712	1.00	51.61
ATOM	912	NH2	ARG	1570	18.824	6.377	21.622	1.00	53.28
ATOM	915 916	C	ARG	1570	20.308	1.023	22.371	1.00	33.90
ATOM	916	0	ARG	1570	21.184	0.391	22.970	1.00	33.17
AION	917	N	GLU	1571	19.359	1.730	22.981	1.00	33.45

217

ATOM 919 CA GLU 1571 19.284 1.861 24.432 1.00 34.87 **ATOM** 920 2.688 1.00 CB GLU 1571 18.052 24.794 35.83 MOTA 921 CG GLU 1571 18.158 4.145 24.354 1.00 41.61 MOTA 922 CDGLU 1571 16.814 4.870 24.318 1.00 47.33 50.68 MOTA 923 OE1 GLU 15.759 1.00 1571 4.199 24.362 MOTA 924 OE2 GLU 1.00 1571 16.812 6.120 24.218 48.07 MOTA 925 GLU 1.00 С 1571 19.223 0.487 25.098 34.39 MOTA 926 0 GLU 1571 19.968 0.202 26.041 1.00 34.04 MOTA 927 N TYR 1572 18.363 -0.376 24.572 1.00 33.49 MOTA 929 CA TYR 1572 -1.728 25.083 18.204 1.00 30.45 MOTA 930 CB TYR 1572 -2.495 24.202 1.00 17.210 28.13 MOTA 931 CG TYR 1572 17.074 -3.971 24.487 1.00 25.80 MOTA 932 CD1 TYR 1572 16.105 -4.443 25.371 1.00 28.92 30.03 ... MOTA 933 CE1 TYR 1572 15.954 -5.804 25.618 1.00 ATOM 934 CD2 TYR 1572 17.899 -4.899 23.863 1.00 24.61 MOTA 935 CE2 TYR 1572 17.760 -6.260 24.102 1.00 26.05 MOTA 936 CZTYR 1572 16.790 -6.705 24.982 1.00 29.23 MOTA 937 OH TYR 1572 16.651 -8.052 25.227 1.00 33.74 MOTA 939 TYR С 1572 19.549 -2.447 25.113 1.00 31.30 MOTA 940 TYR 1572 19.880 -3.126 26.090 0 1.00 32.43 **ATOM** 941 N LEU 1573 20.334 -2.266 24.058 1.00 29.68 **ATOM** 943 LEU 1573 CA 21.625 -2.923 23.972 1.00 30.04 **ATOM** 944 CB LEU 1573 22.145 -2.909 22.529 1.00 26.13 MOTA 945 LEU 1573 25.24 CG -3.870 21.490 21.532 1.00 **MOTA** 946 LEU 1573 CD1 22.097 -3.563 20.113 1.00 19.70 MOTA 947 CD2 LEU 1573 21.807 -5.317 21.839 1.00 22.05 MOTA 948 C LEU 1573 22.645 -2.308 24.927 1.00 34.47 MOTA 949 0 LEU 1573 23.354 -3.031 25.644 1.00 34.95 MOTA 950 N GLN 1574 22.691 -0.980 24.978 1.00 35.47 **ATOM** 952 GLN CA 1574 23.639 -0.293 25.850 1.00 37.09 ATOM 953 GLN CB 1574 23.601 1.206 25.579 1.00 36.70 ATOM 954 CG GLN 1574 1.559 1.00 24.033 24.171 39.77 **ATOM** 955 GLN CD1574 23.960 3.045 23.884 1.00 41.51 MOTA 956 OE1 GLN 1574 23.592 3.837 24.751 1.00 42.57 MOTA 957 NE2 GLN 1574 3.431 22.652 24.288 1.00 41.34 MOTA 960 C GLN 1574 23.400 -0.588 27.332 1.00 37.85 MOTA 961 0 GLN 1574 24.343 -0.801 28.090 1.00 38.87 MOTA 962 N ALA 1575 -0.667 27.720 22.131 1.00 39.01 MOTA 964 CA ALA 1575 -0.944 29.098 21.740 1.00 37.00 MOTA 965 CB ALA 1575 20.261 -0.678 29.273 1.00 35.71 MOTA 966 C ALA 1575 22.061 -2.359 29.559 1.00 39.14 MOTA 967 0 ALA 1575 21.839 -2.692 30.719 1.00 43.81 **ATOM** 968 ARG 1576 38.39 N 22.563 -3.201 28.665 1.00 MOTA 22.897 970 CA ARG 1576 -4.568 29.032 37.71 1.00 **ATOM** 971 ARG 1576 CB 21.994 -5.544 28.290 1.00 38.26 **ATOM** 972 CG ARG 1576 20.555 -5.383 28.700 1.00 38.00 MOTA 973 œ ARG 1576 19.653 -6.282 27.920 1.00 34.74 MOTA 974 NE ARG 1576 18.279 -6.190 28.388 1.00 32.88 MOTA 976 CZARG 1576 17.572 -5.066 28.442 1.00 34.02 MOTA 977 NH1 ARG 1576 18.114 -3.913 28.068 1.00 35.57 MOTA 980 NH2 ARG 1576 16.298 -5.102 28.800 1.00 36.71 MOTA 983 C ARG 1576 24.365 -4.927 28.828 1.00 39.59 MOTA 984 ARG 1576 0 24.735 -6.113 28.788 1.00 39.83 MOTA 985 N ARG 1577 25.200 -3.900 1.00

28.687

38.82

MOTA	987	CA	ARG	1577	26:631	-4.101	28.520	1.00	39.07
ATOM	988	CB	ARG	1577	27.310	-2.797	28.090	1.00	34.91
ATOM	989	CG	ARG	1577	27.033	-2.323	26.681	1.00	33.87
ATOM	990	CD	ARG	1577	27.730	-0.981	26.428	1.00	33.06
ATOM	991	NE	ARG	1577	27.722	-0.612	25.015	1.00	38.87
MOTA	993	CZ	ARG	1577	28.174	0.538	24.517	1.00	39.76
ATOM	994	NH1	ARG	1577	28.683	1.470	25.305	1.00	40.68
MOTA	997	NH2	ARG	1577	28.122	0.758	23.213	1.00	43.26
MOTA	1000	С	ARG	1577	27.181	-4.501	29.885	1.00	41.58
ATOM	1001	0	ARG	1577	26.586	-4.181	30.917	1.00	42.48
ATOM	1002	N	PRO	1578	28.294	-5.249	29.919	1.00	43.07
ATOM	1003	CD	PRO	1578	29.110	-5.812	28.823	1.00	43.36
ATOM	1004	CA	PRO	1578	28.839	-5.626	31.223	1.00	42.69
ATOM	1005	CB	PRO	1578	29.966	-6.595	30.857	1.00	42-22
ATOM	1006	CG	PRO	1578	30.412	-6.103	29.516	1.00	43.64
ATOM	1007	С	PRO	1578	29.366	-4.350	31.882	1.00	43.37
MOTA	1008	o	PRO	1578	29.530	-3.319	31.215	1.00	42.50
MOTA	1009	N	PRO	1579	29.596	-4.380	33.198	1.00	45.24
ATOM	1010	CD	PRO	1579	29.279	-5.435	34.174	1.00	44.69
ATOM	1011	CA	PRO	1579	30.099	-3.187	33.882	1.00	46.27
ATOM	1012	CB	PRO	1579	29.979	-3.567	35.353	1.00	45.78
ATOM	1013	CG	PRO	1579	28.894	-4.615	35.361	1.00	46.15
ATOM	1014	С	PRO	1579	31.548	-2.869	33.500	1.00	48.38
ATOM	1015	0	PRO	1579	32.410	-3.753	33.478	1.00	50.64
ATOM	1016	N	GLU	1592	19.022	-5.398	32.495	1.00	65.98
ATOM	1018	CA	GLU	1592	20.442	-5.048	32.492	1.00	64.80
MOTA	1019	CB	GLU	1592	20.796	-4.241	33.740	1.00	67.30
MOTA	1020	С	GLU	1592	21.351	-6.275	32.371	1.00	63.80
MOTA	1021	0	GLU	1592	22.545	-6.149	32.089	1.00	65.21
ATOM	1022	N	GLU	1593	20.789	-7.458	32.607	1.00	61.44
MOTA	1024	CA	GLU	1593	21.560	-8.691	32.495	1.00	60.82
ATOM	1025	CB	GLU	1593	20.681	-9.899	32.807	1.00	51.47
MOTA	1026	С	GLU	1593	22.144	-8.803	31.089	1.00	59.12
MOTA	1027	0	GLU	1593	21.468	-8.525	30.097	1.00	59.49
ATOM	1028	N	GLN	1594	23.408	-9.201	31.017	1.00	57.33
ATOM	1030	CA	GLN	1594	24.103	-9.334	29 744	1.00	55.30
MOTA	1031	CB	GLN	1594	25.523	- 9.880	29.957	1.00	54.87
ATOM	1032	CG	GLN	1594	26.438	-8. 9 59	30.757	1.00	53.34
ATOM	1033	CD	GLN	1594	27.704	-9.660	31.248	1.00	55.27
MOTA	1034	OE1	GLN	1594	28.256	-10.536	30.572	1.00	56.47
MOTA	1035	NE2	GLN	1594	28.166	-9.275	32.434	1.00	51.46
MOTA	1038	C	GLN	1594	23.336	-10.229	28.781	1.00	52.29
MOTA	1039	0	GLN	1594	22.648	-11.166	29.190	1.00	52.56
MOTA	1040	N	LEU	1595	23.447	-9.913	27.499	1.00	49.40
MOTA	1042	CA	LEU	1595	22.783	-10.676	26.455	1.00	46.00
MOTA	1043	CB	LEU	1595	22.452	-9.760	25.274	1.00	42.94
MOTA	1044	CG.	LEU	1595	21.390	-8.711	25.626	1.00	43.90
MOTA	1045	CD1	LEU	1595	21.495	-7.484	24.743	1.00	39.46
MOTA	1046	CD2	LEU	1595	20.005	-9.347	25.569	1.00	41.86
ATOM	1047	С	LEU	1595	23.741	-11.762	26.029	1.00	43.96
MOTA	1048	О	LEU	1595	24.950	-11.550	26.043	1.00	44.24
ATOM	1049	N	SER	1596	23.217	-12.941	25.714	1.00	43.29
ATOM	1051	CA	SER	1596	24.076	-14.027	25.275	1.00	42.40
ATOM	1052	CB	SER	1596	23.388	-15.374	25.484	1.00	41.83

MOTA 1053 OG SER 1596 22.218 -15.483 24.697 1.00 44.25 MOTA 1055 С SER 1596 24.392 -13.817 23.800 1.00 42.64 MOTA 1056 0 SER 1596 23.857 -12.900 23.171 1.00 43.14 MOTA 1057 N SER 1597 25.277 -14.645 23.255 1.00 42.59 MOTA 1059 CA SER 1597 25.629 -14.553 21.850 1.00 42.91 MOTA 1060 CB SER 1597 26.739 -15.547 21.516 1.00 45.26 MOTA 1061 OG SER 1597 27.812 -15.436 22.431 1.00 56.41 MOTA 1063 C SER 1597 24.380 -14.909 21.048 1.00 42.35 MOTA 1064 0 SER 1597 24.113 -14.322 20.003 1.00 43.71 MOTA 1065 N LYS 1598 23.621 -15.881 21.544 1.00 40.61 MOTA 1067 CA LYS 1598 22.405 -16.298 20.867 1.00 38.61 MOTA 1068 CB LYS 1598 21.848 -17.575 21.483 1.00 36.33 MOTA 1069 CG LYS 1598 21.135 -18.439 20.468 1.00 40.09 ATOM 1070 CD LYS 1598 20.213 __-19.434 21.118 1.00 43.39 ATOM 1071 CE LYS 1598 19.766 -20.494 20.122 1.00 48.25 MOTA 1072 NZ LYS 1598 20.930 -21.290 19.623 1.00 50.46 ATOM 1076 C LYS 1598 21.348 -15.194 20.895 1.00 38.17 MOTA 1077 0 LYS 1598 20.579 -15.053 19.945 1.00 41.27 MOTA 1078 Ŋ ASP 1599 21.321 -14.408 21.969 1.00 35.90 MOTA 1080 CA ASP 1599 20.366 -13.307 22.099 1.00 34.08 MOTA 1081 CB **ASP** 20.450 1599 -12.661 23.477 1.00 37.83 **ATOM** 1082 CG ASP 1599 19.822 -13.505 24.562 1.00 39.93 MOTA 1083 ODI **ASP** 1599 20.089 -13.217 25.742 1.00 45.85 **ATOM** 1084 OD2 ASP 1599 19.060 -14.444 24.240 1.00 41.06 ATOM 1085 C **ASP** 1599 20.634 -12.243 21.061 1.00 32.37 ATOM 1086 o ASP 1599 19.704 -11.701 20.466 1.00 32.58 MOTA 1087 N 21.915 LEU 1600 -11.945 20.873 1.00 30.45 MOTA 1089 CA 1600 -10.948 LEU 22.355 19.902 1.00 29.59 MOTA 1090 CB 1600 LEU 23.841 -10.654 20.097 1.00 28.59 MOTA 1091 CG LEU 1600 24.238 -10.057 21.449 1.00 24.59 MOTA 1092 CD1 LEU 1600 . 25.747 -9.869 21.522 1.00 18.40 MOTA 1093 CD2 LEU 1600 23.529 -8.745 21.626 1.00 21.71 MOTA 1094 C LEU 1600 1.00 22.073 -11.393 18.458 28.54 MOTA 1095 0 LEU 1600 21.578 -10.613 17.648 1.00 25.59 MOTA 1096 N VAL 1601 22.377 -12.645 18.134 1.00 29.13 ATOM 1098 CA VAL 1601 22.111 -13.154 16.793 1.00 29.74 MOTA 1099 CB VAL 1601 22.780 -14.513 16.551 1.00 29.63 MOTA 1100 CG1 VAL 1601 22.615 -14.922 15.105 1.00 29.30 ATOM 1101 CG2 VAL 1601 24.259 -14.422 16.873 1.00 28.52 MOTA 1102 C VAL 1601 20.591 -13.247 16.564 1.00 29.98 VAL MOTA 1103 0 1601 -13.040 20.106 15.452 1.00 29.73 **ATOM** 1104 N SER 1602 -13.493 19.855 17.645 1.00 30.97 MOTA 1106 CA SER 1602 18.399 -13.576 17.607 1.00 29.64 MOTA 1107 CB SER 1602 17.894 -14.141 18.925 1.00 30.45 MOTA 1108 OG SER 1602 16.483 -14.158 18.962 1.00 39.63 MOTA 1110 C SER 1602 17.784 -12.192 17.343 1.00 29.30 MOTA 1111 O SER 1602 16.772 -12.071 16.641 1.00 28.74 MOTA 1112 N CYS 1603 18.385 -11.157 17.925 1.00 27.68 MOTA 1114 CA CYS 1603 17.931 -9.783 17.717 1.00 27.32 MOTA 1115 CB CYS 1603 18.791 -8.790 18.516 1.00 25.40 MOTA 1116 SG CYS 1603 18.472 -7.039 18.177 0.50 20.76 PRT1 MOTA 1117 c CYS 1603 18.057 16.225 -9.468 1.00 28.34 ATOM 1118 0 CYS 1603 17.134 -8.926 15.629 1.00 29.70 MOTA 1119 N ALA 1604 19.192 -9.837 15.627 1.00 29.36

ATOM	1121	CA	ALA	1604	19.438	-9.601	14.195	1.00	28.78
MOTA	1122	CB	ALA	1604	20.861	-10.066	13.808	1.00	22.61
ATOM	1123	С	ALA	1604	18.386	-10.304	13.324	1.00	30.14
ATOM	1124	0	ALA	1604	17.792	-9.690	12.426	1.00	31.64
ATOM	1125	N	TYR	1605	18.156	-11.587	13.605	1.00	29.84
MOTA	1127	CA	TYR	1605	17.179	-12.392	12.874	1.00	28.26
ATOM	1128	CB	TYR	1605	17.107	-13.789	13.488	1.00	28.74
MOTA	1129	CG	TYR	1605	16.018	-14.673	12.912	1.00	31.12
MOTA	1130	CD1	TYR	1605	16.152	-15.256	11.650	1.00	32.53
MOTA	1131	CE1	TYR	1605	15.144	-16.067	11.121	1.00	30.84
ATOM	1132	CD2	TYR	1605	14.853	-14.926	13.634	1.00	31.21
ATOM	1133	CE2	TYR	1605	13.850	-15.734	13.116	1.00	29.69
ATOM	1134	CZ	TYR	1605	14.002	-16.296	11.864	1.00	30.82
ATOM	1135	OH	TYR -	- 1605	12.990	~17.069	11.359	1.00	33.77
MOTA	1137	С	TYR	1605	15.788	-11.758	12.853	1.00	27.33
ATOM	1138	0	TYR	1605	15.152	-11.691	11.805	1.00	27.94
ATOM	1139	N	GLN	1606	15.323	-11.292	14.007	1.00	27.93
MOTA	1141	CA	GLN	1606	14.008	-10.659	14.115	1.00	27.20
MOTA	1142	CB	GLN	1606	13.686	-10.335	15.570	1.00	26.40
ATOM	1143	CG	GLN	1606	13.301	-11.556	16.402	1.00	28.12
MOTA	1144	CD	GLN	1606	13.114	-11.215	17.865	1.00	30.41
MOTA	1145	OE1	GLN	1606	12.188	-10.489	18.234	1.00	34.34
ATOM	1146	NE2	GLN	1606	14.008	-11.701	18.700	1.00	31.44
MOTA	1149	C	GLN	1606	13.906	-9.397	13.275	1.00	29.67
ATOM	1150	0	GLN	1606	12.884	-9.148	12.622	1.00	30.74
ATOM	1151	N	VAL	1607	14.970	-8.602	13.281	1.00	29.59
MOTA	1153	CA	VAL	1607	14.996	-7.377	12.501	1.00	27.00
MOTA	1154	CB	VAL	1607	16.235	-6.544	12.842	1.00	27.20
MOTA	1155	CG1	VAL	1607	16.382	-5.397	11.859	1.00	28.11
MOTA	1156	CG2	VAL	1607	16.113	-5.996	14.266	1.00	24.79
MOTA	1157	C	VAL	1607	14.966	-7. 7 25	11.014	1.00	28.02
MOTA	1158	0	VAL	1607	14.229	-7.108	10.241	1.00	28.28
ATOM	1159	N	ALA	1608	15.736	-8.741	10.626	1.00	27.56
ATOM	1161	CA	ALA	1608	15.787	-9.206	9.236	1.00	27.36
MOTA	1162	CB	ALA	1608	16.801	-10.339	9.095	1.00	26.25
MOTA	1163	С	ALA	1608	14.402	-9.674	8.779	1.00	28.58
MOTA	1164	o	ALA	1608	14.013	-9.446	7.624	1.00	29.11
ATOM	1165	N	ARG	1609	13.660	-10.326	9.680	1.00	28.88
ATOM	1167	CA	ARG	1609	12.306	-10.797	9.376	1.00	27.17
ATOM	1168	CB	ARG	1609	11.797	-11.731	10.464	1.00	29.68
ATOM	1169	CG	ARG	1609	12.458	-13.062	10.439	1.00	31.65
ATOM	1170	CD	ARG	1609	11.612	-14.049	11.177	1.00	38.21
MOTA	1171	NE	ARG	1609	10.856	-14.897	10.269	1.00	41.10
ATOM	1173	CZ	ARG	1609	10.048	-15.872	10.667	1.00	41.97
ATOM	1174	NH1	ARG	1609	9.886	-16.125	11.959	1.00	40.69
ATOM	1177	NH2	ARG	1609	9.411	-16.609	9.770	1.00	43.57
ATOM	1180	C	ARG	1609	11.312	-9.654	9.183	1.00	25.38
ATOM	1181	0	ARG	1609	10.480	-9.693	8.260	1.00	25.75
ATOM	1182	N	GLY	1610	11.365	-8.661	10.070	1.00	24.03
ATOM	1184	CA	GLY	1610	10.480	-7.517	9.939	1.00	21.74
MOTA	1185	C	GLY	1610	10.734	-6.864	8.592	1.00	23.32
ATOM	1186	0	GLY	1610	9.805	-6.540	7.850	1.00	23.39
MOTA	1187	N	MET	1611	12.016	-6.714	8.265	1.00	24.48
ATOM	1189	CA	MET	1611	12.453	-6.125	7.002	1.00	23.13

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ATOM 1611 13.949 -5.860 7.035 1.00 19.46 1190 CB MET MOTA 1191 MET 1611 14.339 -4.671 7.910 1.00 22.46 CG 7.536 **MOTA** 1192 MET 1611 13.457 -3.123 1.00 25.27 SD MOTA 1611 13.900 -2.801 5.876 1.00 22.25 1193 CE MET -7.005 MOTA 1194 C MET 1611 12.100 5.811 1.00 24.87 ATOM 1195 1611 11.699 -6.497 4.755 1.00 24.09 0 MET MOTA 1196 N GLU 1612 12.230 -8.321 5.975 1.00 25.48 MOTA 1198 CA **GLU** 1612 11.894 -9.232 4.890 1.00 25.42 5.288 1.00 MOTA 1199 CB GLU 1612 12.155 -10.691 23.41 MOTA 1200 CG GLU 1612 11.664 -11.679 4.232 1.00 25.14 MOTA 1201 CD GLU 1612 11.872 -13.141 4.599 1.00 28.60 **ATOM** 1202 OE1 GLU 1612 11.637 -13.514 5.777 1.00 30.10 **ATOM** 1203 OE2 GLU 1612 12.244 -13.928 3.694 1.00 29.53 **ATOM** 1204 C GLU 1612 10.418 -9.021 4.521 1.00 26.92 MOTA 1205 GLU 0 1612 10.065 -8.928 3.343 1.00 29.61 MOTA 1206 N TYR 1613 9.576 -8.884 5.542 1.00 27.88 **ATOM** 1208 CA TYR 1613 8.154 -8.675 5.337 1.00 23.B2 **ATOM** 1209 CB TYR 1613 7.415 -8.769 6.667 1.00 24.17 MOTA 1210 CG TYR 1613 5.941 -8.492 6.545 1.00 23.73 **ATOM** 1211 CD1 TYR 1613 5.064 -9.483 6.096 1.00 22.17 ATOM 1212 TYR 1613 3.698 5.965 CE1 -9.235 1.00 21.08 MOTA 1213 CD2 TYR 1613 5.419 -7.237 6.865 1.00 23.16 **ATOM** 1214 CE2 TYR 1613 4.054 -6.976 6.736 1.00 26.38 **ATOM** 1215 CZTYR 1613 3.200 -7.981 6.287 1.00 23.16 MOTA 1216 OH TYR 1613 1.855 -7.725 6.149 1.00 25.50 4.670 **ATOM** 1218 C 1613 7.885 -7.327 1.00 TYR 23.17 MOTA 1219 Э 1613 7.147 -7.246 TYR 3.689 1.00 24.21 MOTA 1220 N LEU 1614 8.481 -6.266 5.206 1.00 23.04 MOTA 1222 CA LEU 1614 8.316 -4.920 4.652 1.00 21.81 MOTA 1223 CB LEU 1614 9.107 -3.906 5.484 1.00 19.94 MOTA 1224 CG 6.902 LEU 1614 8.609 -3.616 1.00 21.94 ATOM 1225 CD1 LEU 1614 9.580 -2.719 7.654 1.00 14.28 MOTA 1226 CD2 LEU 1614 7.227 -2.977 6.814 1.00 17.45 MOTA 1227 C LEU 1614 8.764 -4.858 3.182 1.00 23.74 MOTA 1228 O LEU 1614 8.169 -4.150 2.367 1.00 25.26 MOTA 1229 N ALA 1615 9.831 -5.587 2.862 1.00 25.00 MOTA 1231 CA ALA 1615 10.357 -5.644 1.502 1.00 23.04 ATOM 1232 CB ALA 1615 11.710 -6.360 1.483 1.00 20.02 **ATOM** 1233 C ALA 1615 9.351 -6.357 0.605 1.00 23.15 MOTA 1234 0 ALA 1615 9.076 -5.891 -0.503 1.00 25.25 MOTA 1235 N SER 1616 8.754 -7.441 1.104 1.00 23.64 MOTA 1237 CA SER 1616 7.758 -8.199 1.00 0.337 23.60 **ATOM** 1238 CB SER 1616 7.346 -9.453 1.107 1.00 22.46 MOTA 1239 OG SER 1616 6.531 -9.131 2.224 1.00 26.66 MOTA 1241 C SER 1616 6.505 ~7.369 0.025 1.00 25.45 1.00 MOTA 1242 O SER 1616 5.813 -7.607 -0.967 26.67 **ATOM** 1243 N LYS 1617 6.193 -6.436 0.916 1.00 25.47 MOTA 1245 CA LYS 1617 5.051 -5.551 0.781 1.00 25.04 MOTA 1246 CB LYS 1617 4.513 -5.183 2.163 1.00 26.30 **ATOM** 1247 CG LYS 1617 3.778 -6.318 2.851 1.00 28.58 MOTA 1248 CD LYS 1617 2.438 -6.530 2.169 1.00 33.00 MOTA 1249 CE LYS 1617 1.652 -7.676 2.764 1.00 38.57 MOTA 1250 NZ LYS 1617 2.167 -8.987 2.300 1.00 45.15 MOTA 1254 C LYS 1617 5.417 -4.293 0.002 1.00 26.34

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ATOM	1255	0	LYS	1617	4.649	-3.336	-0.034	1.00	26.77
MOTA	1256	N	LYS	1618	6.592	-4.319	-0.632	1.00	27.17
MOTA	1258	CA	LYS	1618	7.084	-3.197	-1.447	1.00	28.20
MOTA	1259	СВ	LYS	1618	6.053	-2.819	-2.528	1.00	28.42
ATOM	1260	CG	LYS	1618	5.971	-3.749	~3.730	1.00	26.63
ATOM	1261	CD	LYS	1618	5.573	-5.163	-3.364	1.00	30.45
ATOM	1262	CE	LYS	1618	5.636	-6.087	-4.570	1.00	32.50
ATOM	1263	NZ	LYS	1618	4.621	-5.729	-5.600	1.00	34.89
ATOM	1267	С	LYS	1618	7.466	-1.951	-0.643	1.00	28.78
ATOM	1268	0	LYS	1618	7.556	-0.848	-1.199	1.00	28.78
MOTA	1269	N	CYS	1619	7.753	-2.130	0.646	1.00	29.26
ATOM	1271	CA	CYS	1619	8.111	-1.022	1.522	1.00	28.32
MOTA	1272	CB:	CYS	1619	7.391	-1.173	2.873	1.00	26.33
ATOM	1273	SG	CYS		7.754	0.105	4.136	1.00	27.82
MOTA	1274	С	CYS	1619	9.622	-0.841	1.728	1.00	29.15
ATOM	1275	0	CYS	1619	10.336	-1.786	2.072	1.00	29.55
ATOM	1276	N	ILE	1620	10.096	0.378	1.457	1.00	29.39
ATOM	1278	CA	ILE	1620	11.502	0.761	1.625	1.00	27.44
ATOM	1279	СВ	ILE	1620	12.030	1.543	0.381	1.00	25.37
ATOM	1280	CG2	ILE	1620	13.521	1.806	0.506	1.00	19.80
ATOM	1281	CG1	ILE	1620	11.767	0.764	-0.913	1.00	25.40
ATOM	1282	CD1	ILE	1620	12.100	1.557	-2.164	1.00	27.51
ATOM	1283	C	ILE	1620	11.553	1.686	2.855	1.00	26.56
ATOM	1284	0	ILE	1620	11.011	2.792	2.833	1.00	26.68
ATOM	1285	N	HIS	1621	12.193	1.210	3.916	1.00	26.31
ATOM	1287	CA	HIS	1621	12.297	1.967	5.162	1.00	25.00
ATOM	1288	CB	HIS	1621	13.081	1.174	6.210	1.00	23.08
ATOM	1289	CG	HIS	1621	12.848	1.633	7.618	1.00	23.21
ATOM	1290	CD2	HIS	1621	12.224	1.027	8.656	1.00	22.69
ATOM	1291	ND1	HIS	1621	13.260	2.862	8.088	1.00	25.34
ATOM	1293	CE1	HIS	1621	12.909	2.993	9.356	1.00	24.18
ATOM	1294	NE2	HIS	1621	12.273	1.891	9.719	1.00	25.86
MOTA	1296	C	HIS	1621	12.963	3.316	4.976	1.00	25.09
ATOM	1297	0	HIS	1621	12.408	4.328	5.349	1.00	28.21
ATOM	1298	N	ARG	1622.	14.162	3.315	4.402	1.00	26.09
ATOM	1300	CA	ARG	1622	14.976	4.520	4.183	1.00	26.50
ATOM	1301	CB	ARG	1622	14.180	5.670	3.558	1.00	23.52
MOTA	1302	CG	ARG	1622	13.673	5.326	2.202	1.00	23.81
MOTA	1303	CD	ARG	1622	12.995	6.494	1.551	1.00	28.42
ATOM	1304	NE	ARG	1622	12.677	6.170	0.180	1.00	32.52
MOTA	1306	CZ	ARG	1622	11.623	5.455	-0.197	1.00	32.34
MOTA	1307	NHl	ARG	1622	10.774	4.994	0.711	1.00	30.07
ATOM	1310	NH2	ARG	1622	11.460	5.138	-1.489	1.00	28.30
MOTA	1313	C	ARG	1622	15.740	4.993	5.423	1.00	26.31
ATOM	1314	0	ARG	1622	16.698	5.757	5.313	1.00	26.19
ATOM	1315	N	ASP	1623	15.379	4.495	6.596	1.00	27.41
MOTA	1317	CA	ASP	1623	16.114	4.879	7.788	1.00	29.94
ATOM	1318	CB	ASP	1623	15.562	6.155	8.430	1.00	34.83
MOTA	1319	CG	ASP	1623	16.481	6.689	9.533	1.00	38.84
ATOM	1320	OD1	ASP	1623	15.971	7.265	10.514	1.00	44.51
ATOM	1321	OD2	ASP	1623	17.721	6.514	9.423	1.00	37.59
ATOM	1322	С	ASP	1623	16.203	3.763	8.812	1.00	28.71
ATOM	1323	0	ASP	1623	15.845	3.927	9.990	1.00	26.21
MOTA	1324	N	LEU	1624	16.735	2.633	8.357	1.00	26.82

ATOM	1326	CA	LEU	1624	16.905	1.469	9.216	1.00	25.91
ATOM	1327	CB	LEU	1624	17.025	0.209	8.367	1.00	23.35
MOTA	1328	CG	LEU	1624	17.089	-1.107	9.127	1.00	21.09
MOTA	1329	CD1	LEU	1624	15.824	-1.303	10.009	1.00	14.44
MOTA	1330	CD2	LEU	1624	17.282	-2.215	8.101	1.00	18.30
MOTA	1331	C	LEU	1624	18.136	1.640	10.105	1.00	24.93
MOTA	1332	0	LEU	1624	19.235	1.897	9.611	1.00	25.58
MOTA	1333	N	ALA	1625	17.912	1.557	11.416	1.00	26.30
MOTA	1335	CA	ALA	1625	18.945	1.702	12.445	1.00	23.59
ATOM	1336	CB	ALA	1625	19.271	3.174	12.654	1.00	15.82
ATOM	1337	С	ALA	1625	18.351	1.116	13.732	1.00	23.64
ATOM	1338	0	ALA	1625	17.135	0.928	13.825	1.00	26.66
ATOM	1339	N	ALA	1626	19.197	0.815	14712	1.00	21.59
ATOM	1341	CA	ALA	1626	18.708	0.266	15.974	1.00	21.66
ATOM	1342	CB	ALA	1626	19.860	-0.179	16.838	1.00	22.97
ATOM	1343	С	ALA	1626	17.835	1.272	16.731	1.00	24.98
MOTA	1344	0	ALA	1626	17.072	0.891	17.620	1.00	2684
MOTA	1345	N	ARG	1627	17.978	2.558	16.409	1.00	24.55
MOTA	1347	CA	ARG	1627	17.178	3.598	17.942	1.00	25.29
MOTA	1348	CB	ARG	1627	17.699	4.983	16.673	1.00	26.66
ATOM	1349	CG	ARG	1627	17.675	5.276	15.179	1.00	30.56
MOTA	1350	CD	ARG	1627	18.033	6.715	14.902	1.00	34.97
ATOM	1351	NE	ARG	1627	18.177	6.980	13.470	1.00	40.03
MOTA	1353	CZ	ARG	1627	19.322	6.864	12.809	1.00	40.62
ATOM	1354	NH1	ARG	1627	20.421	6.485	13.441	1.00	46.52
MOTA	1357	NH2	ARG	1627	19.377	7.159	11.523	1.00	43.25
ATOM	1360	C	ARG	1627	15.739				

MOTA 1394 CG1 VAL 1631 12.995 -5.469 23.243 1.00 23.92 MOTA 1395 CG2 VAL 1631 14.197 . -3.714 21.895 1.00 24.26 VAL MOTA 1396 C 1631 10.450 -3.773 22.885 1.00 32.64 **ATOM** 1397 0 VAL 1631 10.198 -2.821 23.643 1.00 33.01 ATOM 1398 N THR 1632 9.697 -4.863 22.827 1.00 34.45 MOTA 1400 CA THR 1632 8.516 -5.035 23.660 1.00 34.29 MOTA 1401 CB THR 1632 7.466 -5.941 22.962 1.00 34.62 **ATOM** 1402 OG1 THR 1632 7.965 -7.288 22.881 1.00 34.40 MOTA 1404 CG2 THR 1632 7.154 -5.414 21.551 1.00 31.61 **ATOM** 1405 С THR 1632 8.896 -5.678 24.989 1.00 35.41 ATOM 1406 0 THR 1632 10.002 -6.189 25.146 1.00 34.79 MOTA 1407 Ν GLU 1633 7.939 -5.706 25.913 1.00 36.86 MOTA 1409 CA GLU 1633 8.156 -6.298 27,224 1.00 37.27 ATOM 1410 CB 1633 GLU 6.893 -6.182 28.079 1:00 -37.66 MOTA 1411 CG GLU 1633 7.031 -6.718 29.514 1.00 44.43 MOTA 1412 CD GLU 1633 8.048 -5.**95**9 30.378 1.00 46.68 MOTA 1413 OE1 GLU 1633 8.104 -4.708 30.300 1.00 49.88 MOTA 1414 OE2 GLU 1633 8.783 -6.612 31.156 1.00 48.53 MOTA 1415 C GLU 1633 8.561 -7.753 27.088 1.00 37.15 **ATOM** 1416 0 GLU 1633 9.227 -8.292 27.954 1.00 38.60 MOTA 1417 N **ASP** 1634 8.167 -8.384 25.990 1.00 38.41 ATOM 1419 CA ASP 1634 8.505 -9.787 25.770 1.00 38.86 ATOM 1420 CB ASP 1634 7.381 -10.49925.013 1.00 44.27 **ATOM** 1421 CG ASP 1634 6.022 -10.349 25.690 1.00 50.18 **ATOM** 1422 OD1 ASP 1634 5.726 -11.141 26.617 1.00 52.07 MOTA 1423 OD2 ASP 1634 5.253 -9.439 25.295 1.00 50.17 **ATOM** 1424 C ASP 1634 9.804 -9.947 25.007 1.00 36.23 **ATOM** 1425 0 ASP 1634 10.141 -11.049 24.608 1.00 35.82 MOTA 1426 N ASN 1635 10.528 -8.851 24.799 1.00 36.51 MOTA 1428 CA ASN 1635 11.795 -8.864 24.052 1.00 37.41 **ATOM** 1429 CB ASN 1635 12.801 -9.842 24.678 1.00 38.49 MOTA 1430 CG ASN 1635 13.343 -9.359 26.003 1.00 37.71 **ATOM** 1431 OD1 ASN 1635 13.499 -8.156 26.227 1.00 38.09 ATOM 1432 ND2 ASN 1635 13.679 -10.300 26.874 1.00 39.63 **ATOM** 1435 С ASN 1635 11.655 -9.162 22.552 1.00 36.37 MOTA 1436 0 ASN 1635 12.522 -9.811 21.944 1.00 36.41 MOTA 1437 N VAL 1636 10.547 -8.721 21.966 1.00 33.79 MOTA 1439 CA VAL 1636 10.315 -8.910 20.543 1.00 30.59 MOTA 1440 CB VAL 1636 8.820 -9.139 20.218 1.00 28.83 MOTA 1441 CG1 VAL 1636 8.615 -9.182 18.712 1.00 26.13 ATOM 1442 VAL CG₂ 1636 8.339 -10.431 20.838 1.00 25.67 ATOM 1443 C VAL 1636 10.782 -7.630 19.863 1.00 30.18 MOTA 1444 O VAL 1636 10.436 -6.527 20.301 1.00 27.86 **ATOM** 1445 MET 1637 N 11.609 -7.792 18.832 1.00 30.93 MOTA 1447 CA MET 1637 28.34 12.140 -6.679 18.060 1.00 MOTA 1448 CB MET 1637 13.397 -7.138 17.330 1.00 30.84 MOTA 1449 CG MET 1637 14.480 30.73 -7.693 18.254 1.00 **ATOM** 1450 SD 1637 MET 15.050 -6.490 19.477 1.00 32.20 ATOM 1451 CE MET 1637 15.074 -7.500 20.938 1.00 28.71 MOTA 1452 C MET 1637 11.082 -6.264 17.051 1.00 27.29 **ATOM** 1453 0 MET 1637 10.587 -7.099 16.297 1.00 27.32 ATOM 1454 N LYS 1638 10.733 -4.983 17.045 1.00 27.19 MOTA 1456 CA LYS 1638 9.716 -4.450 16.143 1.00 26.38 **ATOM** 1457 CB LYS 1638 8.437 -4.120 16.912 1.00 27.09

ATOM	1458	CG	LYS	1638	7.702	-5.351	17.407	1.00	29.71
MOTA	1459	CD	LYS	1638	6.386	-5.018	18.109	1.00	31.48
MOTA	1460	CE	LYS	1638	5.485	-6.263	18.202	1.00	27.09
ATOM	1461	NZ	LYS	1638	4.888	-6.561	16.869	1.00	26.6B
ATOM	1465	С	LYS	1638	10.196	-3.208	15.416	1.00	26.56
ATOM	1466	0	LYS	1638	10.514	-2.194	16.040	1.00	27.40
ATOM	1467	N	ILE	1639	10.211	-3.271	14.092	1.00	24.31
ATOM	1469	CA	ILE	1639	10.649	-2.147	13.289	1.00	24.84
ATOM	1470	CB	ILE	1639	10.924	-2.588	11.836	1.00	25.81
MOTA	1471	CG2	ILE	1639	11.248	-1.395	10.952	1.00	24.18
ATOM	1472	CG1	ILE	1639	12.094	-3.566	11.826	1.00	25.01
ATOM	1473	CD1	ILE	1639	12.075	-4.499	10.675	1.00	27.90
MOTA	1474	C	ILE	1639	9.641	-0.999	13.348	1.00	24.90
ATOM	1475	0	ILE	1639	8.435		13.170	1.00	25.24
ATOM	1476	N	ALA	1640	10.167	0.183	13.635	1.00	25.70
MOTA	1478	CA	ALA	1640	9.378	1.392	13.744	1.00	27.61
ATOM	1479	CB	ALA	1640	9.699	2.094	15.070	1.00	26.37
ATOM	1480	С	ALA	1640	9.637	2.348	12.576	1.00	28.35
ATOM	1481	0	ALA	1640	10.650	2.243	11.871	1.00	28.40
MOTA	1482	N	ASP	1641	8.676	3.237	12.354	1.00	29.74
ATOM	1484	CA	ASP	1641	8.760	4.272	11.325	1.00	32.13
ATOM	1485	СВ	ASP	1641	9.873	5.273	11.688	1.00	34.31
ATOM	1486	CG	ASP	1641	9.507	6.158	12.896	1.00	36.31
ATOM	1487	OD1	ASP	1641	10.299	7.056	13.258	1.00	42.18
ATOM	1488	OD2	ASP	1641	8.420	5.974	13.483	1.00	41.03
ATOM	1489	C	ASP	1641	8.882	3.840	9.867	1.00	32.00
ATOM	1490	0	ASP	1641	9.339	4.617	9.021	1.00	32.65
MOTA	1491	N	PHE	1642	8.415	2.634	9.563	1.00	30.61
MOTA	1493	CA	PHE	1642	8.473	2.119	8.200	1.00	30.06
ATOM	1494	CB	PHE	1642	8.248	0.606	8.189	1.00	24.46
MOTA	1495	CG	PHE	1642	6.981	0.176	8.854	1.00	23.26
MOTA	1496	CD1	PHE	1642	5.799	0.075	8.125	1.00	19.66
ATOM	1497	CD2	PHE	1642	6.966	-0.134	10.209	1.00	22.88
ATOM	1498	CE1	PHE	1642	4.609	-0.331	8.734	1.00	20.97
ATOM	1499	CE2	PHE	1642	5.785	-0.540	10.830	1.00	26.61
MOTA	1500	CZ	PHE	1642	4.599	-0.639	10.083	1.00	24.82
ATOM	1501	C	PHE	1642	7.512	2.830	7.225	1.00	33.14
ATOM	1502	0	PHE	1642	7.791	2.922	6.029	1.00	36.48
ATOM	1503	N	GLY	1643	6.411	3.372	7.741	1.00	32.65
ATOM	1505	CA	GLY	1643	5.462	4.059	6.876	1.00	32.28
ATOM	1506	С	GLY	1643	5.629	5.560	6.913	1.00	32.19
MOTA	1507	0	GLY	1643	4.795	6.310	6.415	1.00	30.74
MOTA	1508	N	LEU	1644	6.739	5.997	7.486	1.00	36.80
MOTA	1510	CA	LEU	1644	7.052	7.406	7.630	1.00	41.95
ATOM	1511	CB	LEU	1644	8.332	7.551	8.439	1.00	37.41
ATOM	1512	CG	LEU	1644	8.377	8.746	9.369	1.00	38.98
ATOM	1513	CD1	LEU	1644	7.384	8.548	10.493	1.00	40.45
ATOM	1514	CD2	LEU	1644	9.775	8.904	9.929	1.00	41.94
MOTA	1515	C	LEU	1644	7.189	8.150	6.296	1.00	47.55
MOTA	1516	0	LEU	1644	7.787	7.648	5.341	1.00	50.55
MOTA	1517	N	ALA	1645	6.637	9.356	6.247	1.00	52.59
MOTA	1519	CA	ALA	1645	6.686	10.194	5.055	1.00	56.88
ATOM	1520	CB	ALA	1645	5.391	10.999	4.942	1.00	58.01
ATOM	1521	С	ALA	1645	7.880	11.135	5.178	1.00	58.95
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MOTA 1522 0 ALA 1645 8.064 11:770 6.224 1.00 59.37 MOTA 1523 N ARG 1646 B.700 11.211 4.133 1.00 60.26 **ATOM** 1525 CA ARG 1646 9.870 12.088 1.00 4.165 63.04 **ATOM** 1526 CB ARG 1646 10.995 11.444 4.976 1.00 64.92 ATOM 1527 С ARG 1646 10.377 12.461 2.782 1.00 63.84 MOTA 1528 0 ARG 1646 10.361 11.641 1.864 1.00 63.55 MOTA 1529 N **ASP** 1647 10.801 13.714 2.633 1.00 65.18 **ATOM** 1531 ASP CA 1647 11.332 14.190 1.361 1.00 67.26 MOTA 1532 CB **ASP** 1647 10.989 15.670 1.150 1.00 68.92 MOTA 1533 CG ASP 1647 11.164 16.124 -0.304 1.00 70.88 MOTA 1534 OD1 ASP 1647 12.196 15.811 -0.943 1.00 70.33 MOTA 1535 OD2 ASP 1647 10.258 16.825 -0.808 1.00 71.39 MOTA 1536 C ASP 1647 12.847 14.005 1.405 1.00 68.40 MOTA 1537 0 . . **ASP** 1647 13.545 14.711 2.142 68.66 1.00 **ATOM** 1538 N ILE 1648 13.347 13.055 0.621 1.00 68.48 **ATOM** 1540 CA 1648 14.777 ILE 12.773 0.570 1.00 69.00 MOTA 1541 CB ILE 1648 15.091 11.535 -0.314 1.00 66.28 MOTA 1542 ILE CG2 1648 14.231 10.352 0.131 1.00 65.14 MOTA 1543 CG1 ILE 1648 14.869 11.853 -1.799 1.00 63.01 **ATOM** 1544 CD1 ILE 1648 15.274 10.746 -2.738 1.00 60.11 MOTA 1545 С ILE 1648 15.542 13.990 0.046 1.00 71.12 MOTA 1546 0 ILE 1648 16.628 14.310 0.525 1.00 72.41 **ATOM** 1547 N HIS 1649 14.923 14.710 -0.883 1.00 73.09 MOTA 1549 CA HIS 1649 15.546 15.890 -1.469 1.00 74.66 MOTA 1550 CB HIS 1649 14.921 16.191 -2.835 1.00 76.00 MOTA 1551 15.178 CG HIS 1649 15.157 -3.867 1.00 78.03 MOTA 1552 CD2 HIS 1649 16.314 14.425 -4.151 1.00 78.B5 MOTA 1553 ND1 HIS 1649 14.245 14.739 -4.795 1.00 78.49 MOTA 1555 CEL HIS 1649 14.765 13.835 -5.584 1.00 78.94 MOTA 1556 NE2 HIS 1649 16.005 13.623 -5.226 1.00 78.22 ATOM 1558 C HIS 1649 15.466 17.108 -0.549 1.00 75.04 **ATOM** 1559 0 HIS 1649 15.567 18.244 -1.007 75.49 1.00 1560 MOTA N HIS 1650 15.265 16.860 0.743 1.00 76.11 MOTA 1562 CA HIS 1650 17.918 15.181 1.748 1.00 77.63 MOTA 1563 CB HIS 1650 13.723 18.327 1.995 1.00 81.10 MOTA 1564 CG HIS 1650 13.206 19.352 1.033 1.00 86.06 MOTA 1565 CD2 HIS 1650 13.662 20.592 0.730 1.00 88.74 MOTA 1566 ND1 HIS 1650 12.099 19.146 0.239 1.00 88.83 MOTA 1568 11.893 CE1 HIS 1650 20.211 -0.511 1.00 90.51 MOTA 1569 NE₂ HIS 1650 12.823 21.103 -0.238 1.00 90.75 MOTA 1571 C HIS 1650 15.824 17.482 1.00 3.064 77.39 MOTA 1572 0 HIS 1650 15.651 18.133 4.091 1.00 77.42 MOTA 1573 N ILE 1651 16.573 16.385 3.024 1.00 77.73 MOTA 1575 CA ILE 1651 17.241 15.864 4.212 1.00 77.02 MOTA 1576 CB ILE 1651 17.788 14.433 3.974 1.00 78.24 **ATOM** 1577 ILE 13.963 CG2 1651 18.647 5.153 1.00 77.92 MOTA 1578 CG1 ILE 1651 16.633 13.458 3.750 1.00 80.90 MOTA 1579 CD1 ILE 1651 17.094 12.032 3.483 1.00 82.41 MOTA 1580 C ILE 1651 18.411 16.748 4.620 1.00 76.15 MOTA 1581 ILE 1651 19.269 17.078 1.00 О 3.803 76.52 MOTA 1582 N ASP 1652 18.432 17.150 5.882 1.00 75.13 MOTA 1584 CA ASP 1652 19.527 17.957 6.384 1.00 73.91 ATOM 1585 CB ASP 1652 19.068 18.781 7.592 1.00 76.30 ATOM 1586 CG **ASP** 1652 20.216 19.499 8.286 1.00 79.91

MOTA	1587	OD1	ASP	1652	21.247	19.786	7.636	1.00	B2.38
ATOM	1588	OD2	ASP	1652	20.081	19.780	9.497	1.00	81.51
MOTA	1589	С	ASP	1652	20.637	16.984	6.783	1.00	72.31
ATOM	1590	0	ASP	1652	20.599	16.403	7.866	1.00	71.41
ATOM	1591	N	TYR	1653	21.610	16.805	5.894	1.00	71.44
ATOM	1593	CA	TYR	1653	22.736	15.900	6.143	1.00	70.07
MOTA	1594	CB	TYR	1653	23.655	15.849	4.921	1.00	66.96
ATOM	1595	CG	TYR	1653	23.153	14.932	3.834	1.00	66.43
ATOM	1596	CD1	TYR	1653	23.881	14.757	2.657	1.00	66.60
MOTA	1597	CE1	TYR	1653	23.434	13.898	1.653	1.00	68.33
ATOM	1598	CD2	TYR	1653	21.960	14.224	3.981	1.00	66.58
ATOM	1599	CE2	TYR	1653	21.500	13.363	2.990	1.00	68.84
MOTA	1600	CZ	TYR	1653	22.241	13.205	1.823	1.00	69.34
MOTA	1601	OH	TYR	1653	21.781	12.360	0.833	1.00	69.88
MOTA	1603	С	TYR	1653	23.557	16.227	7.391	1.00	70.80
MOTA	1604	0	TYR	1653	24.197	15.351	7.975	1.00	70.62
MOTA	1605	N	TYR	1654	23.531	17.488	7.802	1.00	70.76
MOTA	1607	CA	TYR	1654	24.280	17.902	8.972	1.00	70.97
ATOM	1608	CB	TYR	1654	24.795	19.328	8.783	1.00	69.27
MOTA	1609	CG	TYR	1654	25.935	19.401	7.787	1.00	69.68
ATOM	1610	CD1	TYR	1654	25.696	19.352	6.415	1.00	69.51
ATOM	1611	CE1	TYR	1654	26.750	19.380	5.498	1.00	70.15
ATOM	1612	CD2	TYR	1654	27.256	19.482	8.221	1.00	69.92
MOTA	1613	CE2	TYR	1654	28.314	19.513	7.316	1.00	70.26
ATOM	1614	CZ	TYR	1654	28.057	19.462	5.958	1.00	70.22
ATOM	1615	OH	TYR	1654	29.111	19.492	5.069	1.00	69.67
ATOM	1617	С	TYR	1654	23.503	17.763	10.272	1.00	72.19
MOTA	1618	0	TYR	1654	24.035	18.043	11.344	1.00	73.21
MOTA	1619	N	LYS	1655	22.269	17.275	10.183	1.00	73.05
MOTA	1621	CA	LYS	1655	21.424	17.108	11.363	1.00	74.81
ATOM	1622	CB	LYS	1655	19.955	17.124	10.953	1.00	75.63
MOTA	1623	CG	LYS	1655	18.978	17.239	12.102	1.00	79.16
ATOM	1624	CD	LYS	1655	17.581	17.513	11.576	1.00	84.09
MOTA	1625	CE	LYS	1655	16.517	17.244	12.634	1.00	87.56
ATOM	1626	NZ	LYS	1655	15.139	17.478	12.097	1.00	89.36
ATOM	1630	С	LYS	1655	21.738	15.834	12.156	1.00	75.72
ATOM	1631	0	LYS	1655	21.900	14.751	11.586	1.00	77.14
ATOM	1632	N	LYS	1656	21.815	15.977	13.477	1.00	75.08
ATOM	1634	CA	LYS	1656	22.106	14.857	14.363	1.00	73.36
ATOM	1635	CB	LYS	1656	23.062	15.296	15.477	1.00	72.88
ATOM	1636	CG	LYS	1656	24.475	15.599	15.007	1.00	72.87
ATOM	1637	CD	LYS	1656	25.346	16.048	16.167	1.00	74.66
ATOM	1638	CE	LYS	1656	26.830	15.945	15.828	1.00	74.84
ATOM	1639	NZ	LYS	1656	27.701	16.322	16.981	1.00	73.74
ATOM	1643	С	LYS	1656	20.827	14.311	14.982	1.00	72.45
ATOM	1644	0	LYS	1656	19.795	14.991	15.007	1.00	72.74
ATOM	1645	N	THR	1657	20.900	13.075	15.469	1.00	71.26
ATOM	1647	CA	THR	1657	19.763	12.426	16.107	1.00	70.05
ATOM	1648	CB	THR	1657	19.969	10.886	16.206	1.00	68.30
ATOM	1649	OG1	THR	1657	21.084	10.598	17.060	1.00	69.34
ATOM	1651	CG2	THR	1657	20.244	10.292	14.839	1.00	66.16
ATOM	1652	C	THR	1657	19.707	13.019	17.504	1.00	70.37
ATOM	1653	0	THR	1657	20.608	13.761	17.892	1.00	71.47
ATOM	1654	N	THR	1658	18.669	12.691	18.263	1.00	70.80

ATOM	1656	CA ·	THR	1658	18.559	13.205	19.626	1.00	71.54
ATOM	1657	CB	THR	1658	17.334	12.600	20.325	1.00	71.20
ATOM	1658	С	THR	1658	19.844	12.865	20.394	1.00	70.91
MOTA	1659	0	THR	1658	20.429	13.722	21.063	1.00	71.25
ATOM	1660	N	ASN	1659	20.331	11.639	20.199	1.00	68.87
MOTA	1662	CA	ASN	1659	21.537	11.157	20.871	1.00	65.52
ATOM	1663	CB	ASN	1659	21.602	9.635	20.796	1.00	67.39
ATOM	1664	CG	ASN	1659	22.419	9.032	21.916	1.00	69.42
ATOM	1665	OD1	ASN	1659	22.261	9.410	23.076	1.00	71.70
MOTA	1666	ND2	ASN	1659	23.278	8.069	21.583	1.00	68.93
ATOM	1669	С	ASN	1659	22.830	11.749	20.318	1.00	62.51
ATOM	1670	0	ASN	1659	23.917	11.351	20.733	1.00	61.47
MOTA	1671	N	GLY	1660	22.706	12.654	19.348	1.00	59.76
MOTA	1673	CA.	GLY	1660	23.859		18.750	1.00	57.70
ATOM	1674	С	GLY	1660	24.553	12.593	17.597	1.00	56.98
ATOM	1675	0	GLY	1660	25.659	12.979	17.199	1.00	57.55
ATOM	1676	N	ARG	1661	23.909	11.573	17.037	1.00	55.34
MOTA	1678	CA	ARG	1661	24.504	10.826	15.928	1.00	52.28
MOTA	1679	СВ	ARG	1661	24.255	9.334	16.092	1.00	50.68
MOTA	1680	CG	ARG	1661	24.811	8.744	17.365	1.00	49.61
ATOM	1681	CD	ARG	1661	24.542	7.267	17.361	1.00	52.30
ATOM	1682	NE	ARG	1661	24.942	6.599	18.595	1.00	53.64
MOTA	1684	CZ	ARG	1661	24.731	5.306	18.826	1.00	56.32
MOTA	1685	NH1	ARG	1661	24.124	4.559	17.901	1.00	54.04
MOTA	1688	NH2	ARG	1661	25.145	4.754	19.965	1.00	54.48
ATOM	1691	С	ARG	1661	24.015	11.288	14.560	1.00	49.89
ATOM	1692	0	ARG	1661	22.916	11.812	14.429	1.00	51.43
ATOM	1693	N	LEU	1662	24.839	11.080	13.542	1.00	45.78
ATOM	1695	CA	LEU	1662	24.503	11.481	12.186	1.00	43.05
ATOM	1696	CB	LEU	1662	25.762	12.020	11.492	1.00	42.15
MOTA	1697	CG	LEU	1662	26.351	13.306	12.088	1.00	40.60
MOTA	1698	CD1	LEU	1662	27.780	13.512	11.641	1.00	38.14
ATOM	1699	CD2	LEU	1662	25.484	14.499	11.705	1.00	42.00
MOTA	1700	С	LEU	1662	23.867	10.346	11.370	1.00	41.81
ATOM	1701	0	LEU	1662	24.548	9.406	10.957	1.00	40.46
ATOM	1702	N	PRO	1663	22.546	10.428	11.118	1.00	40.49
ATOM	1703	CD	PRO	1663	21.659	11.519	11.561	1.00	40.60
ATOM	1704	CA	PRO	1663	21.794	9.423	10.351	1.00	38.17
ATOM	170 5	CB	PRO	1663	20.433	10.095	10.158	1.00	38.43
MOTA	1706	CG	PRO	1663	20.282	10.901	11.414	1.00	40.65
MOTA	1707	С	PRO	1663	22.445	9.059	9.012	1.00	35.40
MOTA	1708	0	PRO	1663	22.265	7.949	8.521	1.00	33.01
ATOM	1709	N	VAL	1664	23.200	9.989	8.426	1.00	34.56
ATOM	1711	CA	VAL	1664	23.889	9.722	7.160	1.00	32.91
MOTA	1712	CB	VAL	1664	24.757	10.916	6.659	1.00	33.13
MOTA	1713	CG1	VAL	1664	23.912	11.929	5.968	1.00	33.44
ATOM	1714	CG2	VAL	1664	25.521	11.554	7.792	1.00	33.68
MOTA	1715	С	VAL	1664	24.812	8.511	7.266	1.00	30.58
MOTA	1716	0	VAL	1664	25.157	7.903	6.257	1.00	29.20
MOTA	1717	N	LYS	1665	25.211	8.171	8.489	1.00	28.02
ATOM	1719	CA	LYS	1665	26.102	7.044	8.726	1.00	24.95
MOTA	1720	CB	LYS	1665	26.749	7.153	10.098	1.00	24.39
MOTA	1721	CG	LYS	1665	27.811	8.231	10.140	1.00	28.36
MOTA	1722	CD	LYS	1665	28.189	8.628	11.548	1.00	29.24

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ATOM 1723 CE LYS 1665 29.269 9.690 11.489 1.00 31.15 12.836 1.00 MOTA 1724 NZ LYS 1665 29.639 10.194 35.47 5.692 8.543 1.00 **ATOM** 1728 C LYS 1665 25.440 25.16 1729 8.627 1.00 **ATOM** LYS 1665 26.096 4.671 24.34 0 5.698 8.286 MOTA 1730 N TRP 1666 24.138 1.00 25.16 ATOM 1732 CA TRP 1666 23.414 4.461 8.053 1.00 26.61 MOTA 1733 CB TRP 1666 22.157 4.412 8.917 1.00 28.17 MOTA 1734 CG TRP 1666 22.428 3.931 10.330 1.00 30.26 MOTA 1735 CD2 TRP 1666 22.930 4.714 11.426 1.00 26.92 **ATOM** 1736 CE2 TRP 1666 23.063 3.837 12.537 1.00 26.34 **ATOM** 1737 CE3 TRP 1666 23.286 6.057 11.598 1.00 24.69 1666 MOTA 1738 CD1 TRP 22.276 2.656 10.800 1.00 26.44 **ATOM** 1739 NE1 TRP 1666 22.659 2.592 12.118 1.00 25.65 MOTA 1741 CZ2 TRP 1666 23.535 4.264 13.779 1.00 24.97 MOTA CZ3 TRP 1742 1666 23.758 6.484 12.837 1.00 22.23 MOTA 1743 CH2 TRP 1666 23.877 5.587 13.908 1.00 24.97 MOTA TRP 23.048 4.345 6.572 1744 C 1666 1.00 27.24 MOTA 1745 0 TRP 1666 22.573 3.301 6.116 1.00 29.16 MOTA 1746 MET 23.355 5.811 N 1667 5.390 1.00 26.70 MOTA 4.398 1748 CA MET 1667 23.022 5.444 1.00 25.21 MOTA MET 3.963 1749 CB 1667 22.828 6.893 1.00 28.81 MOTA 1750 CG MET 1667 21.704 7.630 4.637 1.00 35.42 MOTA 1751 SD MET 1667 21.567 9.283 3.924 1.00 42.64 MOTA 1752 CE MET 1667 20.959 8.858 2.369 1.00 41.32 **MOTA** 1753 С MET 1667 23.984 4.807 3.417 1.00 25.03 MOTA 1754 MET 1667 25.182 5.047 3.446 1.00 O 24.24 MOTA 1755 N ALA 1668 23.420 4.034 2.501 1.00 26.70 MOTA 1757 1.441 27.82 CA ALA 1668 24.186 3.398 1.00 MOTA 1758 CB ALA 1668 23.272 2.509 0.601 1.00 25.36 **ATOM** 1759 1668 24.738 4.528 0.575 1.00 28.42 C ALA **ATOM** 1760 0 ALA 1668 24.044 5.521 0.321 1.00 27.52 MOTA 1761 N PRO 1669 25.972 4.374 0.065 1.00 28.95 MOTA 1762 1669 26.867 3.214 0.170 1.00 27.98 CD **PRO** MOTA 1763 CA PRO 1669 26.571 5.418 -0.775 1.00 28.76 MOTA 1764 CB PRO 1669 27.814 4.731 -1.326 1.00 28.58 MOTA 1765 CG PRO 1669 28.193 3.809 -0.209 1.00 30.22 MOTA 1766 C **PRO** 1669 25.647 5.909 -1.893 1.00 27.08 **MOTA** 1767 7.107 -2.093 0 PRO 1669 25.496 1.00 28.31 ATOM 1768 N GLU 1670 24.993 4.997 -2.595 1.00 25.42 **ATOM** 1770 CA GLU 1670 24.110 5.423 -3.673 1.00 27.02 MOTA 1771 CB GLU 1670 23.680 4.233 -4.542 1.00 27.18 **ATOM** 1772 CG GLU 1670 22.662 3.294 -3.911 1.00 27.66 **MOTA** 1670 1773 CD GLU 23.280 2.162 -3.112 1.00 27.75 **ATOM** 1774 OE1 GLU 1670 22.488 1.309 -2.647 1.00 27.12 MOTA 1775 OE2 GLU 1670 24.526 2.114 -2.944 1.00 21.64 **ATOM** 1776 C GLU 1670 22.896 6.229 -3.189 1.00 26.88 MOTA 1670 7.037 1777 GLU 22.348 -3.929 1.00 0 24.52 MOTA 1778 N ALA 1671 22.477 6.009 -1.948 1.00 29.43 MOTA 1780 ALA 1671 21.342 6.744 -1.392 1.00 CA 29.29 **ATOM** 1781 CB ALA 1671 20.751 5.989 -0.217 1.00 26.98 MOTA 1782 C ALA 1671 21.826 8.124 -0.939 1.00 31.14 MOTA 1783 0 ALA 1671 21.159 9.135 -1.143 1.00 31.67 MOTA 1784 N LEU 1672 23.013 8.139 -0.343 1.00 32.31 MOTA 1786 CA LEU 1672 23.636 9.352 0.154 1.00 33.79

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MOTA 1787 CB LEU 1672 24.841 8.986 1.008 1.00 34.49 ATOM 1788 CG LEU 1672 25.585 10.166 1.618 1.00 37.16 **ATOM** 1789 CD1 LEU 1672 24.713 10.840 2.666 1.00 42.22 MOTA 1790 CD2 LEU 1672 26.863 9.665 2.237 1.00 33.93 **ATOM** 1791 C LEU 1672 24.078 10.280 -0.972 1.00 36.30 **ATOM** 1792 0 LEU 1672 23.789 11.478 -0.949 1.00 39.09 MOTA 1793 N PHE 1673 24.770 9.723 -1.957 1.00 34.39 1795 MOTA CA PHE 1673 25.266 10.504 -3.075 1.00 33.81 MOTA 1796 CB PHE 1673 26.553 9.874 -3.625 1.00 33.15 MOTA 1797 CG PHE 1673 27.661 9.761 -2.617 1.00 33.44 MOTA 1798 CD1 PHE 1673 28.313 8.545 -2.419 1.00 32.17 **MOTA** 1799 CD2 PHE 1673 28.055 10.867 -1.861 1.00 34.87 MOTA 1800 CEl PHE 1673 29:346 8.419 -1.484 1.00 31.98 MOTA - 1801 CE2 PHE 1673 29.090 10.757 - -0.919 1.00 36.31 ATOM 1802 CZPHE 1673 29.736 9.525 -0.732 1.00 34.55 MOTA 1803 C PHE 1673 24.273 -4.217 10.670 1.00 34.79 MOTA 1804 0 PHE 1673 24.135 11.754 -4.765 1.00 35.74 MOTA 1805 N ASP 1674 23.584 9.588 -4.572 1.00 37.31 MOTA 1807 CA ASP 1674 22.650 9.601 -5.698 1.00 35.61 MOTA 1808 CB ASP 1674 22.917 8.392 -6.600 1.00 37.01 MOTA 1809 CG ASP 1674 24.362 8.288 -7.041 1.00 41.02 MOTA 1810 OD1 ASP 1674 25.030 9.340 -7.194 1.00 43.07 MOTA 1811 OD2 ASP 1674 24.828 7.145 -7.251 1.00 42.24 MOTA 1812 C ASP 1674 21.162 9.632 -5.360 1.00 37.06 MOTA 1813 O **ASP** 1674 20.315 9.506 -6.257 1.00 36.37 MOTA 1814 N ARG 1675 20.840 9.745 -4.077 1.00 37.78 ATOM 1816 CA ARG 1675 19.445 9.791 -3.650 1.00 39.41 **ATOM** 1817 CB ARG 1675 18.832 11.137 -4.039 1.00 44.39 **ATOM** 1818 CG ARG 1675 19.413 12.299 -3.269 1.00 54.30 ATOM 1819 CD ARG 1675 19.516 13.551 -4.127 1.00 63.84 ATOM 1820 NE ARG 1675 20.060 14.664 -3.349 1.00 73.69 MOTA 1822 CZ ARG 1675 19.652 15.925 -3.453 1.00 77.10 **ATOM** 1823 NH1 ARG 1675 18.695 16.253 -4.312 1.00 79.65 MOTA 1826 NH2 ARG 1675 20.177 16.855 -2.665 1.00 79.31 ATOM 1829 ARG 1675 18.617 -4.221 C 8.639 1.00 37.46 MOTA 1830 0 ARG 1675 17.447 8.808 -4.557 1.00 38.57 MOTA 1831 N ILE 1676 19.235 7.475 -4.351 1.00 34.37 MOTA 1833 CA ILE 1676 18.545 6.313 -4.874 1.00 32.99 MOTA 1834 CB ILE 1676 19.358 5.644 -5.976 1.00 33.98 **ATOM** 1835 CG₂ ILE 1676 18.552 4.529 -6.602 1.00 35.04 MOTA 1836 CG1 ILE 1676 19.708 6.663 -7.050 1.00 34.92 MOTA 1837 CD1 ILE 1676 20.799 6.200 -7.962 1.00 41.16 **ATOM** 1838 С ILE 1676 18.315 -3.743 1.00 5.315 31.55 MOTA 1839 1676 O ILE 19.245 -3.300 1.00 4.632 30.65 **ATOM** 1840 N TYR 1677 17.082 5.279 -3.246 1.00 30.88 MOTA 1842 CA TYR 1677 16.701 4.371 -2.173 1.00 27.10 MOTA 1843 CB TYR 1677 15.771 5.074 -1.208 1.00 28.30 MOTA 1844 CG TYR 1677 16.457 6.136 -0.406 1.00 30.61 **ATOM** 1845 TYR CD1 1677 16.598 7.432 -0.905 1.00 30.B2 MOTA 1846 CE1 TYR 1677 17.212 8.424 ~0.159 1.00 30.75 **ATOM** 1847 CD2 TYR 1677 16.952 5.857 0.863 1.00 29.75 **ATOM** 1848 CE₂ TYR 1677 17.567 6.842 1.621 1.00 32.62 **ATOM** 1849 CZ TYR 1677 17.688 8.125 1.110 1.00 34.51 **ATOM** 1850 OH TYR 1677 1.888 1.00 18.238 9.118 38.89

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MOTA 1852 С TYR 1677 16.029 3.149 ~2.743 1.00 25.47 MOTA 1853 0 TYR 1677 15.132 3.264 -3.578 1.00 26.00 **ATOM** 1854 N THR 1678 16.459 1.983 -2.272 1.00 24.27 **ATOM** 1856 CA THR 1678 15.942 0.701 -2.734 1.00 24.09 **ATOM** 1857 CB THR 1678 16.830 0.123 -3.853 1.00 24.19 **ATOM** OG1 1858 THR -3.349 1678 18.165 -0.008 1.00 27.81 **ATOM** 1860 CG2 THR 1678 16.843 -5.085 1.00 1.009 24.15 **ATOM** 1861 C THR 1678 15.979 -0.297 -1.577 1.00 25.02 MOTA 1862 0 THR 1678 16.379 0.036 -0.465 1.00 27.65 MOTA 1863 N HIS 1679 15.569 -1.530 -1.844 1.00 25.04 **ATOM** 1865 CA HIS 1679 15.591 -2.560 -0.818 1.00 24.35 **ATOM** 1866 CB HIS 1679 14.853 -3.812 -1.298 1.00 23.78 MOTA 1867 CG HIS 1679 13.390 -3.592 -1.536 1.00 27.24 MOTA 1868 CD2 HIS 1679 12.627 -3.758 -2.643 1.00 28.22 ATOM 1869 ND1 HIS 1679 12.532 -3.137 -0.551 1.00 30.64 **ATOM** 1871 HIS CE1 1679 11.310 -3.028 -1.041 1.00 28.13 MOTA 1872 NE2 HIS 1679 11.339 -3.400 -2.307 1.00 28.52 **ATOM** 1874 С HIS 1679 17.056 -2.846 -0.514 1.00 22.52 MOTA 1875 0 HIS 1679 17.419 -3.179 0.613 1.00 22.58 MOTA 1876 N GLN 1680 -2.604 17.898 -1.516 1.00 24.34 MOTA 1878 CA GLN 1680 19.341 -2.800 -1.406 1.00 23.52 **ATOM** 1879 CB GLN 1680 19.998 -2.781 -2.782 1.00 25.36 MOTA CG 1880 GLN 1680 19.741 -4.050 -3 577 1.00 33.28 ATOM 1881 GLN CD 16B0 19.212 -3.763 -4.949 1.00 34.68 ATOM 1882 OE1 GLN 1680 -5.187 18.683 -2.686 1.00 41.24 ATOM 1883 NE2 GLN 1680 19.357 -4.713 -5.867 1.00 32.10 MOTA 1886 C GLN 1680 19.998 -1.767 ~0.514 1.00 23.38 MOTA 1887 0 GLN 1680 20.925 -2.094 0.224 1.00 25.12 MOTA 1888 N SER 1681 19.533 -0.521 -0.562 1.00 20.87 MOTA 1890 CA SER 1681 20.133 0.480 0.303 1.00 20.53 **ATOM** 1891 CB SER 1681 19.821 1.919 -0.151 1.00 19.58 MOTA 1892 OG SER 1681 18.445 2.126 -0.425 1.00 20.67 ATOM 1894 C SER 1681 19.696 1.741 0.189 1.00 22.22 MOTA 1895 0 SER 1681 20.439 0.455 2.681 1.00 23.62 ATOM 1896 N ASP 1682 18.530 -0.436 1.900 1.00 22.44 ATOM 1898 CA ASP 1682 18.054 -0.816 3.231 1.00 22.70 ATOM 1899 CB ASP 1682 16.607 -1.293 3.180 1.00 24.24 **MOTA** 1900 CG **ASP** 1682 15.603 -0.165 3.352 1.00 28.23 MOTA 1901 OD1 ASP 1682 14.410 -0.425 3.108 1.00 28.14 MOTA 1902 OD2 ASP 1682 15.976 0.960 3.757 1.00 25.23 MOTA 1903 C ASP 1682 18.926 -1.9413.777 1.00 23.92 MOTA 1904 0 ASP 1682 19.121 -2.057 4.990 1.00 26.24 MOTA 1905 N VAL 1683 19.433 -2.788 2.884 1.00 23.67 **ATOM** 1907 CA VAL 1683 20.300 -3.888 3.302 1.00 22.42 MOTA 1908 CB VAL 1683 20.562 -4.881 2.141 1.00 23.70 MOTA 1909 CG1 VAL 1683 21.724 -5.802 2.459 1.00 19.73 MOTA 1910 CG₂ VAL 1683 19.292 -5.713 1.889 1.00 19.85 MOTA 1911 C VAL 1683 21.584 -3.298 3.860 21.94 1.00 1912 MOTA 0 VAL 1683 22.030 -3.688 4.938 1.00 22.69 MOTA 1913 N TRP 1684 22.141 -2.320 3.154 1.00 20.51 MOTA 1915 CA TRP 1684 23.349 -1.633 3.611 1.00 20.31 MOTA 1916 CB TRP 1684 23.659 -0.446 2.680 1.00 19.01 MOTA 1917 CG TRP 1684 24.802 0.410 3.145 1.00 20.67 MOTA 1918 CD2 TRP 1684 26.114 0.468 2.587 1.00 22.26

ATOM 1919 CE2 TRP 1684 26.890 1.316 3.408 1.00 21.22 MOTA 1920 CE3 TRP 1684 26.718 -0.127 1.463 1.00 22.51 ATOM 1921 4.248 1.00 CD1 TRP 1684 24.825 1.229 19.91 MOTA 1922 26.079 1.763 4.414 1.00 NE1 TRP 1684 18.59 MOTA 1924 TRP 1.586 3.148 1.00 CZ2 1684 28.236 20.81 MOTA 1925 CZ3 TRP 1684 28.059 0.141 1.204 1.00 22.01 MOTA 2.047 1926 CH2 TRP 1684 28.806 0.992 1.00 23.34 MOTA 1927 С 5.069 1.00 TRP 1684 23.131 -1.150 21.49 23.34 MOTA 1928 0 TRP -1.412 5.954 1.00 1684 23.958 MOTA 1929 N SER 1685 22.015 -0.463 5.308 1.00 21.84 MOTA 20.02 1931 CA SER 1685 21.652 0.042 6.634 1.00 ATOM 1932 СВ SER 1685 20.310 0.773 6.559 1.00 19.12 MOTA 1933 OG SER 5.578 1.00 21.62 1685 20.335 1.791 ATOM 1935 . . C SER ... 1685 21.551 7.648 1.00 22.64 -1.111 MOTA 1936 0 SER 1685 21.908 -0.946 8.829 1.00 22.09 MOTA 1937 N PHE 1686 21.043 -2.266 7.202 1.00 22.44 CA 1939 8.075 MOTA PHE 1686 20.939 -3.438 1.00 22.91 ATOM 1940 CB PHE 1686 20.196 -4.588 7.380 1.00 23.75 MOTA 1941 CG PHE 1686 -5.808 8.256 1.00 20.027 23.61 MOTA 1942 9.388 CD1 PHE 1686 19.220 -5.757 1.00 21.21 -6.976 MOTA 1943 CD2 PHE 1686 20.731 7.990 1.00 23.91 ATOM 1944 CE1 PHE 1686 19.118 -6.836 10.240 1.00 20.66 MOTA -8.074 8.841 1945 CE₂ PHE 1686 20.636 1.00 22.47 -7.999 MOTA 1946 CZPHE 1686 19.828 9.972 1.00 23.35 -3.904 MOTA 1947 C PHE 1686 22.339 8.522 1.00 22.60 **ATOM** 1948 o PHE 1686 22.526 -4.382 9.646 1.00 22.83 ATOM 1949 N GLY 1687 23.312 -3.770 7.626 1.00 23.82 7.941 MOTA 1951 CA GLY 1687 24.682 -4.140 1.00 22.58 MOTA 1952 С GLY 1687 25.175 -3.262 9.071 1.00 21.49 MOTA 1953 25.832 -3.749 9.990 1.00 21.62 0 GLY 1687 ATOM 9.008 1954 N VAL 1688 24.849 1.968 1.00 21.15 **ATOM** 1956 CA VAL 1688 25.229 -1.008 10.052 1.00 20.56 **ATOM** 9.647 1.00 17.69 1957 CB VAL 1688 24.894 0.479 MOTA VAL 10.690 1.00 15.11 1958 CG1 1688 25.408 1.456 MOTA VÄL B.314 1.00 11.54 1959 CG2 1688 25.518 0.821 -1.398 MOTA 1960 С VAL 1688 24.494 11.346 1.00 22.60 ATOM 1961 25.083 -1.407 12.428 1.00 25.23 0 VAL 1688 MOTA 1962 N LEU 1689 23.215 -1.755 11.229 1.00 26.09 MOTA 1964 CA LEU 1689 22.423 -2.175 12.387 1.00 25.16 MOTA 11.965 1.00 25.91 1965 CB LEU 1689 20.976 -2.455 **ATOM** LEU 13.068 1.00 27.54 1966 CG 1689 19.913 -2.560 MOTA 1967 LEU 12.496 1.00 28.11 CD1 1689 18.557 -2.241 13.704 MOTA 1968 CD2 LEU 1689 19.898 -3.940 1.00 31.67 MOTA 1969 13.018 1.00 27.49 С LEU 1689 23.055 -3.426 ATOM - 1970 · O LEU 23.128 -3.532 14.246 1.00 - 28.99 1689 MOTA 1971 1690 12.180 1.00 27.67 LEU 23.485 -4.374 N MOTA 1973 CA LEU 1690 24.149 -5.596 12.643 1.00 26.76 ATOM 1974 LEU -6.453 11.456 1.00 CB 1690 24.616 28.58 MOTA 1975 CG LEU 1690 23.651 -7.406 10.733 1.00 29.46 MOTA LEU -8.064 9.565 1.00 27.79 1976 CD1 1690 24.372 MOTA 11.691 1.00 1977 CD2 LEU 1690 23.130 -8.488 28.15 MOTA 13.476 1.00 26.19 1978 С LEU 1690 25.362 -5.176 MOTA -5.670 14.597 1.00 25.29 1979 0 LEU 1690 25.565 MOTA 1980 26.124 -4.217 12.946 1.00 25.89 N TRP 1691

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MOTA 1982 CA TRP 1691 27.302 -3.682 13.631 1.00 27.31 MOTA 1983 TRP CB 1691 27.979 -2.628 12.755 1.00 25.21 MOTA 1984 CG TRP 1691 1.00 29.338 -2.170 13.257 27.00 ATOM 1985 CD2 TRP 1691 29.606 -1.060 14.134 1.00 24.28 **ATOM** 1986 CE₂ TRP 1691 31.001 -0.988 14.297 1.00 23.03 MOTA 1987 1691 CE₃ TRP 28.792 -0.118 14.778 1.00 22.80 MOTA 1988 CD1 TRP 1691 30.562 -2.712 12.944 1.00 24.10 MOTA 1989 TRP 1691 NE1 31.557 -2.010 13.567 1.00 23.41 MOTA 1991 CZ2 TRP 1691 31.617 -0.011 15.097 1.00 25.00 **ATOM** 1992 CZ3 TRP 1691 29.398 0.851 15.573 1.00 26.78 ATOM 1993 1691 CH2 TRP 30.802 0.900 15.719 1.00 27.78 MOTA 1994 C TRP 1691 26.947 -3.088 15.012 1.00 28.70 MOTA 1995 O TRP 1691 27.708 15.974 -3.245 1.00 29.56 MOTA 1996 N GLU 1692 25.808 -2.400 15.104 1.00 29.51 MOTA 1998 CA GLU 1692 25.349 -1.817 16.371 1.00 27.55 ATOM 1999 CB GLU 1692 24.120 -0.935 16.171 1.00 28.35 ATOM 2000 CG GLU 1692 24.273 0.221 15.219 1.00 24.70 2001 MOTA CD GLU 1692 22.982 0.989 15.100 1.00 25.44 ATOM 2002 OE1 GLU 1692 22.224 0.744 14.148 1.00 24.34 ATOM 2003 OE₂ GLU 1692 22.696 1.816 15.982 1.00 27.57 MOTA 2004 C GLU 1692 24.958 -2.918 17.352 1.00 28.74 **ATOM** 2005 1692 0 GLU 25.099 -2.753 18.557 1.00 28.76 MOTA 2006 N ILE 1693 24.421 -4.023 16.844 1.00 29.23 MOTA 2008 CA ILE 1693 24.027 -5.125 17.712 1.00 27.48 **ATOM** 2009 CB ILE 1693 23.205 -6.226 16.944 1.00 28.80 ATOM 2010 CG2 ILE 1693 22.983 -7.469 17,842 1.00 22.98 ATOM 2011 CG1 ILE 1693 21.840 -5.658 16.508 1.00 27.36 MOTA 2012 CD1 ILE 1693 21.005 -6.585 15.635 1.0C 24.84 **ATOM** 2013 1693 C ILE 25.259 -5.750 1.00 18.357 27.27 **ATOM** 2014 ILE 1693 0 25.320 -5.902 19.575 1.00 28.15 **ATOM** 2015 PHE 1694 N 26.273 -6.043 17.552 1.00 27.83 MOTA 2017 CA PHE 1694 27.473 -6.677 18.095 1.00 29.88 **ATOM** 2018 CB PHE 1694 28.143 -7.525 17.011 1.00 28.66 MOTA 2019 CG PHE 1694 27.223 -8.574 16.463 1.00 29.92 **ATOM** 2020 CD1 PHE 1694 26.628 -8.424 15.220 1.00 30.20 MOTA 2021 CD2 PHE 1694 26.809 -9.630 17.269 1.00 30.81 MOTA 2022 CE1 PHE 1694 25.625 -9.294 14.801 1.00 32.42 MOTA 2023 CE2 PHE 1694 25.805 -10.508 16.857 1.00 32.30 MOTA 2024 CZ 1694 PHE 25.210 -10.337 15.628 1.00 31.13 **MOTA** 2025 C PHE 1694 28.429 -5.784 18.890 1.00 31.07 MOTA 2026 0 PHE 1694 29.376 -6.273 19.509 1.00 33.16 MOTA 2027 1695 N THR 28.157 -4.480 18.897 1.00 29.20 MOTA 2029 CA THR 1695 28.934 -3.532 1.00 19.670 27.38 ATOM 2030 CB THR 1695 29.412 1.00 -2.333 18.823 24.77 MOTA 2031 OG1 THR 1695 28.287 -1.652 18.274 1.00 26.27 MOTA 2033 CG2 THR 1695 30.305 -2.800 1.00 17.706 20.18 MOTA 2034 C THR 1695 28.053 -3.034 20.822 1.00 29.84 **ATOM** 2035 О THR 1695 28.430 -2.103 21.548 1.00 32.77 MOTA 2036 N LEU 1696 1.00 26.898 -3.687 20.988 28.52 MOTA 2038 CA LEU 1696 25.915 -3.364 22.029 1.00 28.82 MOTA 2039 CB LEU 1696 26.356 -3.886 23.394 1.00 32.50 MOTA 2040 CG LEU 1696 26.658 -5.379 23.476 1.00 33.24 **ATOM** 2041 1696 CD1 LEU 27.205 -5.717 24.849 1.00 34.15 ATOM 2042 CD2 LEU 1696 25.398 -6.150 23.191 1.00 37.24

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ATOM 2043 С LEU 1696 25.553 -1.888 22.131 1.00 26.98 MOTA 2044 0 LEU 1696 25.579 -1.297 23.207 1.00 27.59 **ATOM** 2045 1697 N GLY 25.148 -1.317 21.007 1.00 27.86 MOTA 2047 CA GLY 1697 24.767 0.074 20.980 1.00 27.40 MOTA 2048 C GLY 1697 25.927 0.962 20.618 1.00 27.47 **ATOM** 2049 0 GLY 1697 25.957 2.132 20.998 1.00 28.78 ATOM 2050 N GLY 1698 26.888 0.416 19.885 1.00 27.26 **ATOM** 2052 CA GLY 1698 28.031 1.212 19.482 1.00 29.54 **ATOM** 2053 С GLY 1698 27.651 2.301 18.492 1.00 31.17 **ATOM** 2054 0 GLY 1698 26.669 2.177 17.755 1.00 33.73 MOTA 2055 N SER 1699 28.418 3.380 18.481 1.00 29.96 ATOM 2057 CA SER 1699 28.168 4.491 17.577 1.00 29.37 MOTA 2058 CB SER 1699 28.438 5.810 18.319 1.00 31.77 MOTA 2059 OG .. SER 1699 28.575 6.919 17.431 1.00 38.42 MOTA 2061 C SER 1699 29.093 4.350 16.369 1.00 27.98 MOTA 2062 0 SER 1699 30.299 4.310 16.529 1.00 28.18 MOTA 2063 N PRO 1700 28.537 4.240 15.153 1.00 29.62 MOTA 2064 CD PRO 1700 27.104 4.259 14.794 1.00 31.22 MOTA 2065 CA **PRO** 1700 29.381 4.107 13.958 1.00 28.95 MOTA 2066 CB PRO 1700 28.356 4.003 12.807 1.00 27.21 MOTA 2067 CG PRO 1700 27.095 3.556 13.460 1.00 29.33 MOTA 2068 С PRO 1700 30.205 5.379 13.773 1.00 28.78 ATOM 2069 0 PRO 1700 29.737 6.469 14.110 1.00 30.04 MOTA 2070 N TYR 1701 31.426 5.239 13.264 1.00 28.35 MOTA 2072 CA TYR 1701 32.296 6.390 12.987 1.00 30.77 MOTA 2073 CB TYR 1701 31.921 6.987 11.615 1.00 31.67 MOTA 2074 CG TYR 1701 32.060 6.037 10.454 1.00 34.61 MOTA 2075 CD1 TYR 1701 30.952 5.673 9.686 1.00 38.26 MOTA 2076 CE1 TYR 1701 31.083 4.806 8.587 1.00 40.99 ATOM 2077 CD2 TYR 1701 33.301 5.520 10.106 1.00 38.16 MOTA 207B CE2 TYR 1701 33.449 4.662 9.020 1.00 41.04 MOTA 2079 CZTYR 1701 32.343 4.312 8.263 1.00 43.11 MOTA 2080 OH TYR 1701 32.531 3.478 7.181 1.00 49.53 MOTA 2082 C 1701 TYR 32.305 7.532 14.029 1.00 31.41 MOTA 2083 0 TYR 1701 32.026 8.689 13.698 1.00 33.59 MOTA 2084 N PRO 1702 32.635 7.230 15.296 1.00 30.92 MOTA 2085 CD PRO 1702 32.998 5.938 15.888 1.00 32.30 MOTA 2086 CA PRO 1702 32.656 8.283 16.314 1.00 30.05 MOTA 2087 CB PRO 1702 33.123 7.548 17.561 1.00 27.77 MOTA 2088 CG PRO 1702 32.676 6.174 17.338 1.00 32.34 **ATOM** 2089 C 1702 PRO 33.659 9.366 15.944 1.00 31.42 MOTA 2090 0 PRO 1702 34.769 9.055 15.513 1.00 30.95 **ATOM** 2091 N GLY 1703 33.257 10.627 16.117 1.00 31.30 **ATOM** 2093 GLY CA 1703 34.122 11.751 15.817 1.00 29.66 2094 MOTA С GLY 1703 34.172 12.138 14.351 1.00 31.00 MOTA 2095 0 GLY 1703 34.752 13.165 13.999 1.00 30.69 MOTA 2096 N VAL 1704 33.551 11.331 13.491 1.00 31.11 MOTA 2098 CA VAL 1704 33.553 11.610 12.059 1.00 29.88 MOTA 2099 CB VAL 1704 33.539 10.310 11.244 1.00 28.41 MOTA 2100 CG1 VAL 1704 33.585 10.624 9.750 1.00 26.24 MOTA 2101 CG2 VAL 1704 34.702 9.429 11.649 1.00 24.10 MOTA 2102 C 1704 32.396 VAL 12.508 11.604 1.00 30.80 MOTA 2103 0 VAL 1704 31.224 12.146 11.712 1.00 32.50

2104

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PRO

1705

32.718

13.705

11.104

1.00

30.86

MOTA

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ATOM 2105 . CD 1705 34.039 PRO 14.350 11.077 1.00 30.59 **ATOM** 2106 CA 1705 PRO 31.682 14.625 10.645 1.00 31.47 **ATOM** 2107 CB **PRO** 1705 32.400 15.971 10.680 1.00 32.75 ATOM 2108 1705 CG PRO 33.774 15.607 10.289 1.00 32.59 **ATOM** 2109 C PRO 1705 31.258 14.264 9.239 1.00 32.19 MOTA 2110 0 PRO 1705 31.974 13.536 8.549 1.00 33.91 MOTA 2111 N VAL 1706 30.124 14.814 8.806 1.00 32.57 MOTA 2113 CA VAL 1706 29.560 14.576 7.474 1.00 31.80 **ATOM** 2114 CB VAL 1706 28.483 15.632 7.172 1.00 34.66 MOTA 2115 CG1 VAL 1706 28.022 15.538 5.738 1.00 39.06 MOTA 2116 VAL CG2 1706 27.309 15.455 8.106 1.00 36.62 MOTA 2117 С VAL 1706 30.578 14.560 6.320 1.00 31.58 MOTA 2118 0 , VAL 1706 30..682 13.585 5.570 1.00 32.35 MOTA 2119 N GLU 1707 31.326 15.649 6.189 1.00 31.46 **ATOM** 2121 CA GLU 1707 32.329 15.788 5.139 1.Õ0 31.68 ATOM 2122 CB GLU 1707 33.021 17.148 5.267 1.00 32.59 MOTA 2123 С GLU 1707 33.381 14.678 5.114 1.00 32.23 MOTA 2124 0 GLU 1707 33.740 14.183 4.050 1.00 33.47 **ATOM** 2125 N GLU 1708 33.902 14.316 6.279 1.CO 32.90 MOTA 2127 CA GLU 1708 34.909 13.268 6.352 1.00 33.86 **ATOM** 2128 CB GLU 1708 35.570 13.244 7.730 1.00 38.54 **ATOM** 2129 CG GLU 1708 36.190 14.575 8.165 1.00 47.63 MOTA 2130 GLU CD 1708 37.442 14.962 7.383 1.00 58.35 ATOM 2131 OE1 GLU 1708 38.117 14.067 6.816 1.00 62.88 MOTA 2132 OE2 GLU 1708 37.770 16.176 7.355 1.00 64.79 MOTA 2133 C GLU 1708 34.276 11.921 6.043 1.00 33.56 **ATOM** 2134 0 GLU 1708 34.927 11.038 5.489 1.00 34.18 MOTA 2135 N LEU 1709 32.997 11.774 6.374 1.00 32.91 **MOTA** 2137 CA LEU 1709 32.285 10.532 6.108 1.00 33.83 MOTA 2138 CB LEU 1709 30.862 10.563 6.685 1.00 32.28 ATOM 2139 CG LEU 1709 30.015 9.363 6.231 1.00 32.92 ATOM 2140 LEU CD1 1709 30.541 8.071 6.853 1.00 28.37 ATOM 2141 CD2 LEU 1709 28.563 9.580 6.568 1.00 31.90 ATOM 2142 C, LEU 1709 32.222 10.283 4.606 1.00 34.15 MOTA 2143 0 LEU 1709 32.412 9.152 4.156 1.00 34.75 MOTA 2144 N PHE 1710 31.918 11.332 3.844 1.00 33.83 MOTA 2146 CA PHE 1710 31.828 11.248 2.388 1.00 32.90 MOTA 2147 СB PHE 1710 31.531 12.622 1.787 1.00 34.85 ATOM 2148 CG PHE 1710 30.162 13.132 2.082 1.00 38.60 ATOM 2149 CD1 PHE 1710 29.150 12.268 2.469 1.00 43.69 MOTA 2150 CD2 PHE 1710 29.882 14.480 1.984 1.00 45.10 **ATOM** 2151 CEl PHE . 1710 27.873 12.742 2.764 1.00 46.23 **ATOM** 2152 CE2 PHE 1710 28.611 14.966 2.274 1.00 48.15 MOTA 2153 CZ PHE 1710 27.603 14.086 2.670 1.00 46.90 **ATOM** 2154 С PHE 1710 33.131 10.739 1.803 1.00 31.84 MOTA 2155 0 PHE 1710 33.134 9.931 0.877 1.00 29.97 MOTA 2156 N LYS 1711 34.231 11.224 2.373 1.00 32.45 MOTA 2158 CA LYS 1711 35.582 10.860 1.947 1.00 34.53 MOTA 2159 CB LYS 1711 36.588 11.755 2.675 1.00 36.17 **ATOM** 2160 CG LYS 1711 38.008 11.669 2.182 1.00 41.07 **ATOM** 2161 CDLYS 1711 38.912 12.582 3.001 1.00 46.23 ATOM 2162 CE LYS 1711 40.311 12.648 2.418 1.00 51.79 MOTA 2163 NZ LYS 1711 41.036 11.360 2.556 1.00 57.27 MOTA 2167 С LYS 1711 35.867 9.375 2.215 1.00 33.82

MOTA	2168	0	LYS	1711	36.451	8.688	1.376	1.00	33.20
MOTA	2169	N	LEU	1712	35.439	8.885	3.382	1.00	34.52
ATOM	2171	CA	LEU	1712	35.618	7.477	3.754	1.00	33.25
ATOM	2172	CB	LEU	1712	35.094	7.211	5.189	1.00	30.99
MOTA	2173	CG	LEU	1712	35.746	7.917	6.393	1.00	29.71
MOTA	2174	CD1	LEU	1712	35.047	7.552	7.678	1.00	24.11
MOTA	2175	CD2	LEU	1712	37.208	7.552	6.497	1.00	32.21
MOTA	2176	С	LEU	1712	34.833	6.631	2.744	1.00	32.16
ATOM	2177	0	LEU	1712	35.378	5.732	2.109	1.00	32. 7 7
MOTA	2178	N	LEU	1713	33.562	6.967	2.563	1.00	31.72
ATOM	2180	CA	LEU	1713	32.700	6.259	1.637	1.00	33.60
ATOM	2181	СВ	LEU	1713	31.299	6.879	1.619	1.00	36.57
ATOM	2182	CG	LEU	1713	30.522	6.711	2.930	1.00	37.60
ATOM	2183	CD1	LEU	1713	29.284	7.575	2.927	1.90	35.03
ATOM	2184	CD2	LEU	1713	30.182	5.246	3.157	1.00	33.22
ATOM	2185	С	LEU	1713	33.285	6.248	0.236	1.00	35.33
ATOM	2186	O	LEU	1713	33.318	5.203	-0.407	1.00	36.00
ATOM	2187	N	LYS	1714	33.741	7.405	-0.234	1.00	36.24
ATOM	2189	CA	LYS	1714	34.331	7.501	-1.566	1.00	36.35
ATOM	2190	СВ	LYS	1714	34.707	8.946	-1.900	1.00	35.82
ATOM	2191	CG	LYS	1714	33.520	9.837	-2.168	1.00	37.23
ATOM	2192	CD	LYS	1714	32.712	9.324	-3.337	1.00	
ATOM	2193	CE	LYS	1714	31.506	10.198	-3.609	1.00	40.53 44.51
ATOM	2194	NZ	LYS	1714	30.747	9.724	-4.804	1.00	
ATOM	2198	c	LYS	1714	35.559	6.613	-1.701	1.00	50.76
ATOM	2199	Ö	LYS	1714	35.808	6.039	-2.764	1.00	37.60 40.82
ATOM	2200	N	GLU	1715	36.299	6.452	-0.615	1.00	35.61
ATOM	2202	CA	GLU	1715	37.496	5.630	-0.658	1.00	34.65
ATOM	2203	СВ	GLU	1715	38.517	6.188	0.320	1 00	37.83
ATOM	2204	CG	GLU	1715	38.897	7.613	-0.036	1.00	42.28
ATOM	2205	CD	GLU	1715	39.634	8.342	1.061	1.00	
ATOM	2206	OE1	GLU	1715	39.928	7.726	2.114	1.00	45.64
ATOM	2207	OE2	GLU	1715	39.918	9.544	0.853	1.00	43.09
ATOM	2208	C	GLU	1715	37.244	4.145	~0.419	1.00	47.56 32.94
ATOM	2209	o	GLU	1715	38.177	3.348	-0.419	1.00	
ATOM	2210	N	GLY	1716	35.983	3.779	-0.213	1.00	33.31
ATOM	2212	CA	GLY	1716	35.634	2.391	0.004		29.12
ATOM	2213	C.	GLY	1716	35.946	1.895	1.396	1.00 1.00	26.02
ATOM	2214	ō	GLY	1716	36.223	0.715	1.588	1.00	29.60
ATOM	2215	N	HIS	1717	35.879	2.783	2.379	1.00	29.81
ATOM	2217	CA	HIS	1717	36.158	2.409	3.763		29.97
ATOM	2218	CB	HIS	1717	36.369	3.659	4.623	1.00	30.78
ATOM	2219	CG	HIS	1717	36.653	3.360	6.067	1.00	33.25
ATOM	2220	CD2	HIS	1717				1.00	34.70
ATOM	2221	ND1	HIS	1717	37.820	3.155	6.715	1.00	32.77
ATOM	2223	CE1	HIS		35.656	3.219	7.010	1.00	36.90
ATOM	2224			1717	36.200	2.932	8.180	1.00	35.87
ATOM	2224	NE2	HIS	1717	37.513	2.887	8.027	1.00	31.93
ATOM		C	HIS	1717	35.035	1.577	4.375	1.00	29.63
	2227	0	HIS	1717	33.861	1.847	4.133	1.00	30.82
ATOM	2228	N	ARG	1718	35.406	0.600	5.201	1.00	27.92
ATOM	2230	CA	ARG	1718	34.436	-0.258	5.878	1.00	27.30
MOTA	2231	CB	ARG	1718	34.379	-1.641	5.236	1.00	24.10
ATOM	2232	CG	ARG	1718	33.939	-1.655	3.789	1.00	26.52
ATOM	2233	CD	ARG	1718	32.469	-1.288	3.627	1.00	26.96

MOTA 2234 NE ARG 1718 32.020 -1.374 2.232 1.00 24.41 **ATOM** 2236 CZARG 1718 32.090 -0.377 1.352 1.00 25.51 MOTA 2237 NH1 ARG 1718 32.611 0.801 1.706 1.00 23.61 **ATOM** 2240 NH2 ARG 1718 31.553 -0.521 0.149 1.00 21.28 MOTA 2243 C ARG 1718 34.881 -0.384 7.330 1.00 28.81 MOTA 2244 0 ARG 1718 36.080 -0.425 7.611 1.00 29.77 ATOM 2245 N MET 1719 33.920 -0.377 8.250 1.00 30.40 ATOM 2247 CA MET 1719 34.215 -0.485 9.673 1.00 30.62 ATOM 2248 CB MET 1719 32.942 -0.339 10.497 1.00 28.91 MOTA 2249 CG MET 1719 32.235 1.003 10.316 1.00 30.85 MOTA 2250 SD MET 1719 30.829 1.237 11.432 1.00 33.27 **ATOM** 2251 CE MET 1719 29.521 0.416 10.561 1.00 31.81 **ATOM** 1719 , 2252 C MET 34.900 -1.793 10.005 1.00 31.32 **ATOM** 2253 О MET 1719 34.755 -2.769 9.278 1.00 31.47 ATOM 2254 N ASP 1720 35.651 -1.799 11.103 1.00 33.78 **ATOM** 2256 CA ASP 1720 36.387 -2.983 11.550 1.00 33.45 MOTA 2257 CB ASP 1720 37.478 -2.580 12.546 1.00 36.99 ATOM 2258 CG ASP 1720 38.585 -1.762 11.908 1.00 41.56 MOTA 2259 OD1 ASP 1720 38.403 -1.339 10.742 1.00 48.43 **ATOM** 2260 OD2 **ASP** 1720 39.634 -1.546 12.568 1.00 40.99 MOTA 2261 C ASP 1720 35.473 -4.001 12.211 1.00 32.12 MOTA 2262 o ASP 1720 34.381 -3.657 12.668 1.00 30.89 MOTA 2263 N LYS 1721 35.944 -5.241 12.328 1.00 31.82 MOTA 2265 35.127 CA LYS 1721 -6.270 12.953 1.00 31.71 MOTA 2266 CB LYS 1721 35.691 -7.679 12.747 1.00 32.34 **MOTA** 2267 CG LYS 1721 34.762 -8.738 13.344 1.00 34.85 **ATOM** 2268 CD LYS 1721 35.111 -10.155 12.961 1.00 37.39 **ATOM** 2269 CE LYS 1721 35.266 -10.674 13.765 1.00 41.42 MOTA 2270 ÑΖ LYS 1721 36.348 -12.154 13.635 1.00 46..55 ATOM 2274 C LYS 1721 35.007 -6.018 14.430 1.00 33.40 MOTA 2275 0 LYS 1721 36.017 -5.879 15.121 1.00 34.26 MOTA 2276 N PRO 1722 33.768 -5.924 14.934 1.00 34.26 MOTA 2277 CD PRO 1722 32.494 -6.002 14.203 1.00 32.16 MOTA 2278 CA PRO 1722 33.546 -5.692 16.362 1.00 35.84 MOTA 2279 CB PRO 1722 32.027 -5.682 16.473 1.00 35.35 MOTA 2280 CG PRO 1722 31.575 -5.255 15.108 1.00 35.35 MOTA 2281 C PRO 1722 34.105 -6.904 17.099 1.00 40.41 MOTA 2282 0 1722 PRO 34.010 -8.038 16.607 1.00 41.14 MOTA 2283 N SER 1723 34.739 -6.680 1.00 18.240 43.60 MOTA 2285 CA SER 1723 35.260 -7.808 18.999 1.00 45.51 MOTA 2286 CB SER 1723 36.078 -7.324 20.191 1.00 45.30 MOTA 2287 OG 1723 SER 35.384 -6.300 20.879 1.00 49.62 MOTA 2289 С SER 1723 34.031 -8.589 19.460 1.00 46.39 **ATOM** 2290 0 SER 1723 32.939 -8.028 19.614 1.00 45.16 MOTA 2291 N ASN 1724 34.199 -9.891 19.631 1.00 48.53 MOTA 2293 CA ASN 1724 33.088 -10.723 20.065 1.00 51.13 MOTA 2294 CB ASN 1724 32.509 -10.194 21.390 1.00 56.87 ATOM 2295 ASN CG 1724 33.595 -9.892 22.427 1.00 61.65 **ATOM** 2296 OD1 ASN 1724 34.503 -10.702 22.649 1.00 63.73 MOTA 2297 ND2 ASN 1724 33.526 -8.713 23.039 1.00 64.64 MOTA 2300 C ASN 1724 32.034 -10.743 18.941 1.00 48.83 MOTA 2301 0 ASN 1724 30.846 -10.534 19.145 1.00 50.50 **MOTA** 2302 N **CYS** 1725 32.511 -10.977 17.734 1.00 45.23 **ATOM** 2304 CA CYS 1725 31.654 -11.056 16.570 1.00 42.33

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ATOM 2305 CB CYS 1725 31.570 -9.702 15.854 1.00 41.48 **MOTA** 2306 SG **CYS** 1725 30.711 -9.751 14.275 1.00 40.38 **ATOM** 2307 С CYS 1725 32.383 -12.077 15.725 1.00 39.64 MOTA 2308 0 CYS 1725 33.601 -12.004 15.579 1.00 42.00 MOTA 2309 N THR 1726 31.664 -13.090 15.263 1.00 35.96 **ATOM** 2311 CA THR 1726 32.275 -14.139 14.459 1.00 33.61 MOTA 2312 CB THR 1726 31.301 -15.326 14.326 1.00 33.29 **MOTA** 2313 OG1 THR 1726 30.071 -14.904 13.711 1.00 34.53 2315 1726 MOTA CG2 THR 30.981 -15.861 15.696 1.00 25.84 MOTA 2316 C THR 1726 32.720 -13.629 13.092 1.00 32.27 MOTA 2317 0 THR 1726 32.257 -12.593 12.643 1.00 33.04 **ATOM** 2318 N ASN 1727 33.643 -14.315 12.434 1.00 32.98 **MOTA** 2320 CA ASN 1727 34.050 -13.850 11.114 1.00 34.97 **ATOM** 2321 CB ASN 1727 35.198 -14.680 10:541 1.00 39.89 ATOM 2322 CG ASN 1727 36.540 -14.271 1.00 11.103 45.37 **ATOM** 2323 OD1 ASN 1727 37.044 -13.177 10.826 1.00 48.43 ND2 MOTA 2324 ASN 1727 37.125 -15.141 11.909 1.00 45.88 **ATOM** 2327 C ASN 1727 32.846 -13.947 10.192 1.C0 33.97 ATOM 2328 О ASN 1727 32.646 -13.088 9.341 1.00 35.07 N . MOTA 2329 GLU 1728 32.024 -14.973 10.414 1.00 31.69 MOTA 2331 CA GLU 1728 30.B14 -15.210 9.620 1 00 30.27 **ATOM** 2332 -16.493 CB GLU 1728 30.141 10.083 1.00 32.53 MOTA 2333 ÇG GLU 1728 28.932 -16.878 9.273 1.00 32.81 MOTA 2334 CD GLU 1728 28.353 -18.190 9.711 1.00 36.43 MOTA 2335 OE1 GLU 1728 28.339 -18.466 10.932 1.00 36.75 MOTA 2336 OE2 GLU 1728 27.908 -18.945 8.823 1.00 41.92 MOTA 2337 C. GLU 1728 29.814 -14.049 9 681 1.00 28.70 MOTA 2338 0 GLU 1728 29.234 -13.655 8.660 1.00 28.51 MOTA 2339 N LEU 1729 29.594 -13.517 10.880 1.00 26.77 MOTA 2341 CA LEU 1729 28.687 -12.393 11.040 1.00 26.80 MOTA 2342 CB LEU 1729 28.228 -12.274 12.490 1.00 27.91 MOTA 2343 CG LEU 1729 27.233 -13.355 12.913 1.00 30.71 MOTA 2344 CD1 LEU 1729 27.095 -13.345 14.428 1.00 35.79 MOTA 2345 CD2 LEU 1729 25.885 -13.141 12.253 1.00 25.70 MOTA 2346 С LEU 1729 29.319 -11.089 10.540 1.00 27.06 MOTA 2347 0 LEU 1729 28.610 -10.177 10.126 1.00 30.27 MOTA 2348 N TYR 1730 30.650 -11.004 10.549 1.00 27.03 MOTA 2350 CA TYR 1730 31.328 -9.812 10.039 1.00 26.21 MOTA 2351 CB TYR 1730 32.792 -9.778 10.474 1.00 25.31 **ATOM** 33.538 2352 CG TYR 1730 -8.553 9.982 1.00 24.89 ATOM 2353 CD1 TYR 33.012 1730 -7.270 10.169 1.00 23.59 MOTA 2354 CE1 TYR 33.655 1730 -6.148 9.665 1.00 24.74 MOTA 2355 CD2 TYR 1730 34.739 -8.675 9.285 1.00 22.11 MOTA 2356 CE2 TYR 1730 35.399 -7.560 8.775 1.00 22.32 MOTA 2357 CZ TYR 1730 34.853 -6.295 8.962 1.00 26.07 MOTA 2358 OH TYR 1730 35.484 -5.181 8.418 1.00 22.70 MOTA 2360 С 1730 31.227 TYR -9.878 8.509 1.00 27.71 **ATOM** 2361 0 1730 TYR 30.960 -8.875 7.843 1.00 28.05 MOTA 2362 N MET 1731 31.409 -11.081 7.977 1.00 27.92 **ATOM** 2364 CA MET 1731 31.306 -11.355 6.548 1.00 28.89 MOTA 2365 MET 31.506 CB 1731 -12.853 6.317 1.00 35.84 MOTA 2366 CG MET 1731 31.068 -13.379 4.975 1.00 45.50 MOTA 2367 SD MET 1731 31.347 -15.167 4.865 1.00 56.40 ATOM 2368 CE MET 1731 32.106 -15.263 3.217 1.00 56.88

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ATOM	2369	С	MET	1731	29.916	-10.928	6.102	1.00	27.79
ATOM	2370	Ο	MET	1731	29.755	-10.345	5.041	1.00	30.68
ATOM	2371	N	MET	1732	28.915	-11.203	6.932	1.00	28.02
MOTA	2373	CA	MET	1732	27.546	-10.804	6.639	1.00	25.74
ATOM	2374	CB	MET	1732	26.598	-11.317	7.718	1.00	24.94
MOTA	2375	CG	MET	1732	25.153	-10.911	7.492	1.00	22.96
ATOM	2376	SD	MET	1732	24.008	-11.593	8.684	1.00	24.39
ATOM	2377	CE	MET	1732	23.798	-13.272	8.002	1.00	18.04
MOTA	2378	C	MET	1732	27.470	-9.273	6.559	1.00	25.81
MOTA	2379	0	MET	1732	26.889	-8.729	5.620	1.00	26.85
ATOM	2380	N	MET	1733	28.068	-8.587	7.537	1.00	24.84
ATOM	2382	CA	MET	1733	28.092	-7.124	7.545	1.00	25.27
MOTA	2383	CB	MET	1733	28.931	-6.600	9.700	1.00	25.97
MOTA	2384	CG	MET	1733	28.342	-6.769	10.058	1.00	28.69
MOTA	2385	SD	MET	1733	29.456	-6.094	11.295	1.00	29.06
ATOM	2386	CE	MET	1733	28.927	-7.051	12.693	1.00	28.07
ATOM	2387	C	MET	1733	28.741	-6.628	6.270	1.00	26.97
ATOM	2388	0	MET	1733	28.192	-5.771	5.581	1.00	28.37
ATOM	2389	N	ARG	1734	29.922	-7.160	5.966	1.00	28.77
ATOM	2391	CA	ARG	1734	30.664	-6.775	4.762	1.00	29.66
ATOM	2392	CB	ARG	1734	32.027	-7.482	4.716	1.00	29.05
ATOM	2393	CG	ARG	1734	32.968	-7.109	5.866	1.00	25.00
MOTA	2394	CD	ARG	1734	33.247	-5.621	5.882	1.00	29.27
MOTA	2395	NE	ARG	1734	33.911	-5.210	4.647	1.00	35.43
MOTA	2397	CZ	ARG	1734	35.233	-5.220	4.466	1.00	38.24
MOTA	2398	NH1	ARG	1734	36.054	-5.601	5.445	1.00	36.47
MOTA	2401	NH2	ARG	1734	35.732	-4.967	3.277	1.00	38.57
ATOM	2404	С	ARG	1734	29.859	-7.034	3.478	1.00	29.57
MOTA	2405	0	ARG	1734	29.920	-6.242	2.538	1.00	29.55
ATOM	2406	N	ASP	1735	29.095	-8.124	3.448	1.00	28.07
MOTA	2408	CA	ASP	1735	28.259	-8.423	2.287	1.00	27.96
ATOM	2409	CB	ASP	1735	27.634	-9.813	2.408	1.00	28.60
ATOM	2410	CG	ASP	1735	28.664	-10.926	2.283	1.00	31.34
ATOM	2411	OD1	ASP	1735	29.785	-10.660	1.798	1.00	31.12
ATOM	2412	OD2	ASP	1735	28.356	-12.068	2.687	1.00	36.07
ATOM	2413	С	ASP	1735	27.159	-7.368	2.155	1.00	27.24
ATOM	2414	0	ASP	1735	26.846	-6.932	1.050	1.00	25.79
ATOM	2415	N	CYS	1736	26.590	-6.951	3.288	1.00	26.53
ATOM	2417	CA	CYS	1736	25.547	-5.930	3.314	1.00	24.35
ATOM	2418	CB	CYS	1736	24.968	-5.765	4.731	1.00	22.01
ATOM	2419	SG	CYS	1736	23.885	-7.101	5.281	1.00	21.52
ATOM	2420	C	CYS	1736	26.119	-4.595	2.847	1.00	24.26
ATOM	2421	0	CYS	1736	25.386	-3.725	2.368	1.00	24.19
MOTA	2422	N	TRP	1737	27.432	-4.437	3.002	1.00	22.94
ATOM	2424	CA	TRP	1737	28.104	-3.210	2.605	1.00	21.91
ATOM	2425	CB	TRP	1737	29.146	-2.820	3.640	1.00	19.26
ATOM	2426	CG	TRP	1737	28.572	-2.493	4.947	1.00	20.89
ATOM	2427	CD2	TRP	1737	29.226	-2.602	6.212	1.00	23.33
ATOM	2428	CE2	TRP	1737	28.315	-2.159	7.196	1.00	21.59
ATOM	2429	CE3	TRP	1737	30.506	-3.026	6.614	1.00	25.00
ATOM	2430	CD1	TRP	1737	27.319	-2.012	5.201	1.00	19.90
ATOM	2431	NE1	TRP	1737	27.158	-1.807	6.551	1.00	20.77
ATOM	2433	CZ2	TRP	1737	28.641	-2.127	8.563	1.00	19.89
MOTA	2434	CZ3	TRP	1737	30.825	-2.993	7.971	1.00	21.23

MOTA	2435	CH2	TRP	1737	29.896	-2.543	8.927	1.00	21.09
MOTA	2436	С	TRP	1737	28.758	-3.266	1.232	1.00	23.54
MOTA	2437	0	TRP	1737	29.653	-2.477	0.939	1.00	24.68
ATOM	2438	N	HIS	1738	28.315	-4.185	0.382	1.00	24.37
ATOM	2440	CA.	HIS	1738	28.877	-4.287	-0.947	1.00	24.42
ATOM	2441	CB	HIS	1738	28.243	-5.436	-1.728	1.00	23.72
ATOM	2442	CG	HIS	1738	29.131	-5.985	-2.801	1.00	27.20
ATOM	2443	CD2	HIS	1738	29.595	-5.425	-3.948	1.00	26.45
ATOM	2444	ND1	HIS	1738	29.681	-7.255	-2.751	1.00	29.26
ATOM	2446	CE1	HIS	1738	30.436	-7.441	-3.816	1.00	29.25
MOTA	2447	NE2	HIS	1738	30.409	-6.358	-4.556	1.00	27.32
ATOM	2449	C	HIS	1738	28.716	-2.970	-1.713	1.00	25.82
ATOM	2450	O	HIS	1738	27.675	-2.314	-1.660	1.00	23.96
ATOM	2451	N	ALA	1739	29.802	-2.564	-2.362	1.00	26.27
ATOM	2453	CA	ALA	1739	29.825	-1.346	-3.158	1.00	25.46
ATOM	2454	CB	ALA	1739	31.186	-1.180	-3.789	1.00	25.70
ATOM	2455	С	ALA	1739	28.754	-1.443	-4.233	1.00	26.18
MOTA	2456	0	ALA	1739	28.116	-0.455	-4.574	1.00	29.14
ATOM	2457	N	VAL	1740	28.570	-2.643	-4.774	1.00	25.71
ATOM	2459	CA	VAL	1740	27.560	-2.875	-5.802	1.00	26.12
ATOM	2460	CB	VAL	1740	28.063	-3.841	-6.903	1.00	25.99
ATOM	2461	CG1	VAL	1740	27.102	-3.832	-8.090	1.00	23.37
ATOM	2462	CG2	VAL	1740	29.450	-3.440	-7.349	1.00	22.07
ATOM	2463	C	VAL	1740	26.247	-3.400	-5.191	1.00	25.43
ATOM	2464	0	VAL	1740	26.186	-4.550	-4.704	1.00	24.93
MOTA	2465	N	PRO	1741	25.170	-2.585	-5.265	1.00	24.20
ATOM	2466	CD	PRO	1741	25.151	-1.277	-5.953	1.00	18.88
ATOM	2467	CA	PRO	1741	23.838	-2.914	-4.734	1.00	25.28
ATOM	2468	CB	PRO	1741	22.953	-1.788	-5.294	1.00	22.75
ATOM	2469	CG	PRO	1741	23.903	-0.632	-5.398	1.00	20.99
MOTA	2470	C	PRO	1741	23.299	-4.296	-5.128	1.00	25.84
MOTA	2471	е	PRO	1741	22.787	-5.036	-4.280	1.00	25.99
MOTA	2472	N	SER	1742	23.425	-4.642	-6.407	1.00	26.48
MOTA	2474	CA	SER	1742	22.942	-5.919	-6.930	1.00	25.19
MOTA	2475	CB	SER	1742	23.151	-5.992	-8.440	1.00	25.68
MOTA	2476	OG	SER	1742	24.530	-5.943	-8.769	1.00	27.46
MOTA	2478	C	SER	1742	23.644	-7.100	-6.289	1.00	25.24
ATOM	2479	0	SER	1742	23.124	-8.218	-6.300	1.00	26.09
ATOM	2480	N	GLN	1743	24.826	-6.851	-5.731	1.00	23.88
MOTA	2482	CA	GLN	1743	25.590	-7.917	-5.118	1.00	24.44
ATOM	2483	CB	GLN	1743	27.069	-7.733	-5.437	1.00	27.26
MOTA	2484	CG	GLN	1743	27.344	-7.784	-6.940	1.00	27.39
ATOM	2485	CD	GLN	1743	26.803	-9.047	-7.581	1.00	26.46
MOTA	2486	OE1	GLN	1743	27.325	-10.136	-7.339	1.00	25.80
MOTA	2487	NE2	GLN	1743	25.760	-8.914	-8.393	1.00	27.42
MOTA	2490	С	GLN	1743	25.348	-8.151	-3.633	1.00	23.20
ATOM	2491	0	GLN	1743	25.810	-9.147	-3.083	1.00	22.90
ATOM	2492	N	ARG	1744	24.628	-7.243	-2.984	1.00	22.15
ATOM	2494	CA	ARG	1744	24.318	-7.398	-1.568	1.00	21.23
ATOM	2495	СВ	ARG	1744	23.767	-6.088	-0.998	1.00	19.01
ATOM	2496	CG	ARG	1744	24.705	-4.916	-1.145	1.00	17.27
ATOM	2497	CD	ARG	1744	24.091	-3.605	-0.679	1.00	14.79
ATOM	2498	NE	ARG	1744	24.914	-2.493	-1.157	1.00	19.72
ATOM	2500	CZ	ARG	1744	24.482	-1.258	-1.391	1.00	19.23
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ATOM	2501	.NH1	ARG	1744	23.201	-0.931	-1.201	1.00	15.90
MOTA	2504	NH2	ARG	1744	25.343	-0.343	-1.821	1.00	19.43
ATOM	2507	C	ARG	1744	23.259	-8.496	-1.438	1.00	21.95
ATOM	2508	0	ARG	1744	22.585	-8.827	-2.415	1.00	25.34
ATOM	2509	N	PRO	1745	23.213	-9.184	-0.292	1.00	20.82
ATOM	2510	CD	PRO	1745	24.191	-9.219	0.804	1.00	21.25
MOTA	2511	CA	PRO	1745	22.204	-10.229	-0.127	1.00	21.39
ATOM	2512	СВ	PRO	1745	22.687	-10.980	1.117	1.00	21.69
MOTA	2513	CG	PRO	1745	23.418	-9.916	1.886	1.00	22.62
MOTA	2514	C	PRO	1745	20.833	-9.585	0.102	1.00	22.15
MOTA	2515	0	PRO	1745	20.739	-8.402	0.426	1.00	23.29
ATOM	2516	N	THR	1746	19.771	-10.349	-0.109	1.00	20.93
ATOM	2518	CA	THR	1746	18.440	-9.827	0.107	1.00	19.90
ATOM	2519	CB	THR	1746	17.391	-10.554	-0.783	1.00	20.21
ATOM ATOM	2520 2522	OG1 CG2	THR THR	1746	17.484	-11.974	-0.584	1.00	22.03
ATOM	2523	C	THR	1746 1746	17.609	-10.242	-2.255	1.00	20.82
ATOM	2524	0	THR	1746	18.112 18.842	-10.095	1.557	1.00	19.77
ATOM	2525	N	PHE	1747		-10.823	2.228	1.00	19.19
ATOM	2527	CA	PHE	1747	17.010 16.582	-9.526 -9.770	2.045	1.00	23.46
ATOM	2528	CB	PHE	1747	15.473	-8.794	3.422 3.827	1.00	21.64
ATOM	2529	CG	PHE	1747	15.987	-7.445	4.262	1.00	18.89 17.45
ATOM	2530	CD1	PHE	1747	16.757	-7.317	5.417	1.00	17.45
ATOM	2531	CD2	PHE	1747	15.712	-6.303	3.516	1.00	15.37
ATOM	2532	CEI	PHE	1747	17.242	-6.073	5.819	1.00	16.17
ATOM	2533	CE2	PHE	1747	16.189	-5.056	3.907	1.00	14.53
ATOM	2534	CZ	PHE	1747	16.959	-4.941	5.065	1.00	16.98
ATOM	2535	C	PHE	1747	16.118	-11.227	3.522	1.00	23.18
ATOM	2536	0	PHE	1747	16.271	-11.873	4.548	1.00	24.04
MOTA	2537	N	LYS	1748	15.570	-11.745	2.432	1.00	24.13
ATOM	2539	CA	LYS	1748	15.137	-13.132	2.385	1.00	26.35
MOTA	2540	CB	LYS	1748	14.502	-13.424	1.024	1.00	27.52
ATOM	2541	CG	LYS	1748	14.034	-14.849	0.836	1.00	33.88
ATOM	2542	CD	LYS	1748	13.598	-15.062	-0.600	1.00	41.83
ATOM	2543	CE	LYS	1748	13.190	-16.506	-0.881	1.00	50.05
MOTA	2544	NZ	LYS	1748	12.084	-16.986	0.005	1.00	55.70
MOTA	2548	С	LYS	1748	16.359	-14.037	2.636	1.00	27.50
ATOM	2549	0	LYS	1748	16.303	-14.950	3.459	1.00	31.18
ATOM	2550	Ŋ	GLN	1749	17.467	-13.761	1.949	1.00	27.24
ATOM	2552	CA	GLN	1749	18.699	-14.529	2.122	1.00	27.03
MOTA	2553	CB	GLN	1749	19.797	-14.039	1.169	1.00	31.80
ATOM	2554	CG	GLN	1749	19.501	-14.196	-0.323	1.00	38.57
MOTA MOTA	2555	CD	GLN	1749	20.460	-13.385	-1.209	1.00	39.93
ATOM	2556 2557	OE1 NE2	GLN	1749	20.025	-12.535	-1.974	1.00	39.90
ATOM		C	GLN	1749	21.768	-13.620	-1.068	1.00	40.23
ATOM	2560		GLN	1749	19.205	-14.380	3.552	1.00	25.98
ATOM	2561 2562	О И	GLN LEU	1749 1750	19.533 19.293	-15.371	4.198	1.00	27.18
ATOM	2562 2564	CA	LEU	1750	19.293	-13.133 -12.823	4.018	1.00	25.20
ATOM	2565	CB	LEU	1750	19.774	-12.823	5.369	1.00	25.74
ATOM	2566	CG	LEU	1750	20.708	-11.317	5.631 4.831	1.00	20.99
ATOM	2567	CD1	LEU	1750	20.708	-8.987	4.831	1.00	20.90
ATOM	2568	CD2	LEU	1750	20.302	-10.643	5.426	1.00	19.88
ATOM	2569	C	LEU	1750	18.985	-13.555	6.441	1.00	17.26 27.10
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ATOM	2570	0	LEU	1750	19.553	-14.094	7.392	1.00	27.89
ATOM	2571	N	VAL	1751	17.672	-13.598	6.265	1.00	29.40
ATOM	2573	CA	VAL	1751	16.798	-14.262	7.210	1.00	26.80
MOTA	2574	CB	VAL	1751	15.324	-14.030	6.843	1.00	26.94
MOTA	2575	CG1	VAL	1751	14.429	-14.941	7.657	1.00	29.93
MOTA	2576	CG2	VAL	1751	14.941	-12.575	7.117	1.00	24.10
MOTA	2577	С	VAL	1751	17.136	-15.745	7.228	1.00	27.80
MOTA	2578	0	VAL	1751	17.223	-16.359	8.285	1.00	26.77
MOTA	2579	N	GLU	1752	17.408	-16.300	6.056	1.00	32.26
MOTA	2581	CA	GLU	1752	17.749	~17.717	5.966	1.00	35.72
ATOM	2582	CB	GLU	1752	17.721	-18.173	4.504	1.00	39.33
ATOM	2583	CG	GLU	1752	16.306	-18.078	3.911	1.00	49.41
MOTA	2584	CD	GLU	1752	16.209	-18.421	2.429	1.00	55.88
MOTA	2585	OE1	GLU	1752	15.141	-18.138	1.835	1.00	58.00
ATOM	2586	OE2	GLU	1752	17.180	-18.978	1.863	1.00	61.03
MOTA	2587	С	GLU	1752	19.093	-18.002	6.635	1.00	34.59
ATOM	2588	0	GLU	1752	19.230	-18.975	7.393	1.00	33.95
ATOM	2589	N	ASP	1753	20.057	-17.114	6.401	1.00	34.38
MOTA	2591	CA	ASP	1753	21.393	-17.235	6.977	1.00	32.81
MOTA	2592	CB	ASP	1753	22.338	-16.227	6.334	1.00	31.57
ATOM	2593	CG	ASP	1753	22.628	-16.556	4.888	1.00	33.68
MOTA	2594	ODJ	ASP	1753	22.573	-17.755	4.536	1.00	35.14
MOTA	2595	OD2	ASP	1753	22.914	-15.624	4.104	1.00	34.44
MOTA	2596	C	ASP	1753	21.378	-17.058	8.489	1.00	32.04
ATOM	2597	O	ASP	1753	21.997	-17.837	9.214	1.00	31.21
ATOM	2598	N	LEU	1754	20.648	-16.045	8.955	1.00	31.00
MOTA	2600	CA	LEU	1754	20.528	-15.754	10.382	1.00	29.46
MOTA	2601	СВ	LEU	1754	19.822	-14.426	10.598	1.00	23.47
ATOM	2602	CG	LEU	1754	20.816	-13.309	10.318	1.00	23.58
ATOM	2603	CD1	LEU	1754	20.114	-11.963	10.128	1.00	20.46
MOTA	26C4	CD2	LEU	1754	21.828	-13.282	11.462	1.00	19.18
MOTA	2605	C	LEU	1754	19.806	-16.866	11.110	1.00	31.84
MOTA	2606	0	LEU	1754	20.125	-17.178	12.254	1.00	30.78
ATOM ATOM	2607	N C2	ASP	1755	18.832	-17.471	10.445	1.00	34.03
ATOM	2609 2610	CA	ASP	1755	18.116	-18.578	11.044	1.00	35.22
ATOM	2611	CB CG	ASP ASP	1755	16.973 16.159	-19.027	10.148	1.00	38.40
ATOM	2612	OD1	ASP	.1755 1755	15.560	-20.119 -19.866	10.779 11.841	1.00 1.00	41.85
ATOM	2613	OD1	ASP	1755	16.142	-21.241	10.238	1.00	47.90 46.67
ATOM	2614	C	ASP	1755	19.114	-19.724	11.222	1.00	36.79
ATOM	2615	c	ASP	1755		-20.411	12.250	1.00	38.33
ATOM	2616	N	ARG	1756	19.973	-19.920	10.226	1.00	34.81
MOTA	2618	CA	ARG	1756	20.982	-20.969	10.302	1.00	34.68
ATOM	2619	CB	ARG	1756	21.688	-21.100	8.959	1.00	34.78
MOTA	2620	CG	ARG	1756	22.746	-22.179	8.910	1.00	35.93
ATOM	2621	CD	ARG	1756	23.297	-22.306	7.511	1.00	41.60
ATOM	2622	NE	ARG	1756	23.786	-21.025	6.999	1.00	46.42
ATOM	2624	CZ	ARG	1756	24.889	-20.419	7.427	1.00	48.38
ATOM	2625	NHl	ARG	1756	25.637	-20.976	8.381	1.00	48.10
ATOM	2628	NH2	ARG	1756	25.236	-19.242	6.909	1.00	46.62
ATOM	2631	С	ARG	1756	22.002	-20.666	11.399	1.00	36.17
ATOM	2632	0	ARG	1756	22.372	-21.541	12.177	1.00	38.33
ATOM	2633	N	ILE	1757	22.433	-19.413	11.478	1.00	37.00
ATOM	2635	CA	ILE	1757	23.416	-18.998	12.468	1.00	35.60

ATOM	2636	CB	ILE	1757	23.964	-17.588	12.141	1.00	35.54
ATOM	2637	CG2	ILE	1757	24.921	-17.131	13.217	1.00	32.41
ATOM	2638	CG1	ILE	1757	24.693	-17.612	10.794	1.00	
ATOM	2639	CD1	ILE	1757	25.097	-16.253	10.287	1.00	33.49
ATOM	2640	C.	ILE	1757	22.866	-19.048	13.891	1.00	37.28
ATOM	2641	0	ILE	1757	23.531	-19.556	14.779	1.00	38.42
MOTA	2642	N	VAL	1758	21.634	-18.585	14.088	1.00	39.19
ATOM	2644	CA	VAL	1758	21.016	-18.584	15.421	1.00	
MOTA	2645	CB	VAL	1758	19.560	-18.017	15.403	1.00	
MOTA	2646	CG1	VAL	1758	18.918	-18.144	16.773	1.00	38.30
MOTA	2647	CG2	VAL	1758	19.560	-16.560	15.009	1.00	
ATOM	2648	С	VAL	1758	20.983	-19.997	15.988	1.00	41.98
ATOM	2649	0	VAL	1758	21.380.	-20.229	17.128	1.00	43.36
ATOM	2650	N	ALA	1759	20.501	-20.932	15.182	1.00	43.31
ATOM	2652	CA	ALA	1759	20.418	-22.325	15.589	1.00	44.00
MOTA	2653	СВ	ALA	1759	19.836	-23.150	14.459	1.00	44.52
MOTA	2654	С	ALA	1759	21.784	-22.867	15.976	1.00	45.98
MOTA	2655	0	ALA	1759	21.894	-23.725	16.841	1.00	48.78
MOTA	2656	N	LEU	1760	22.823	-22.375	15.319	1.00	48.93
ATOM	2658	CA	LEU	1760	24.175	-22.831	15.592	1.00	51.47
ATOM	2659	CB	LEU	1760	24.954	-22.900	14.280	1.00	53.63
ATOM	2660	CG	LEU	1760	24.284	-23.864	13.295	1.00	57.84
MOTA	2661	CD1	LEU	1760	24.993	-23.847	11.948	1.00	61.83
ATOM	2662	CD2	LEU	1760	24.260	-25.277	13.886	1.00	58.57
MOTA	2663	С	LEU	1760	24.911	-21.965	16.607	1.00	53.60
MOTA	2664	0	LEU	1760	26.078	-22.214	16.919	1.00	54.00
MOTA	2665	N	THR	1761	24.222	-20.963	17.141	1.00	55.77
ATOM	2667	CA	THR	1761	24.820	-20.060	18.111	1.00	56.64
ATOM	2668	CB	THR	1761	24.250	-18.627	17.979	1.00	55.76
ATOM	2669	OG1	THR	1761	24.444	-18.154	16.644	1.00	56.20
ATOM	2671	CG2	THR	1761	24.962	-17.680	18.917	1.00	55.25
MOTA	2672	С	THR	1761	24.636	-20.548	19.539	1.00	58.16
ATOM	2673	0	THR	1761	23.566	-21.021	19.919	1.00	56.85
ATOM	2674	N	SER	1762	25.706	-20.436	20.318	1.00	61.74
MOTA	2676	CA	SER	1762	25.706	-20.833	21.717	1.00	64.50
ATOM	2677	CB	SER	1762	27.155	-20.979	22.205	1.00	68.82
MOTA	2678	OG	SER	1762	27.232	-21.544	23.508	1.00	73.15
MOTA	2680	С	SER	1762	24.965	-19.775	22.547	1.00	63.87
ATOM	2681	0	SER	1762	25.080	-18.563	22.296	1.00	63.22
ATOM	3420	PA	PCP	400	62.748	10.301	7.817	1.00	90.90
ATOM	3421	Ola	PCP	400	62.509	10.036	9.280		92.35
ATOM	3422	02A	PCP	400	61.832	11.180	7.038	1.00	90.49
ATOM	3423	05*	PCP	400	62.744	8.904	7.142	1.00	83.57
ATOM	3424	PB	PCP	400	65.226	11.946	8.294	1.00	
ATOM	3425	01B	PCP	400	65.246	13.015	7.264	1.00	102.85
ATOM	3426	02B	PCP	400	66.527	11.458	8.830	1.00	99.88
ATOM	3427	03A	PCP	400	64.334	10.725	7.584	1.00	96.64
ATOM	3428	C3B	PCP	400	64.345	12.502	9.635	1.00	102.94
ATOM	3429	C5*	PCP	400	62.337	8.684	5.839	1.00	71.21
ATOM	3430	C4*	PCP	400	62.479	7.204	5.587	1.00	64.48
ATOM	3431	04*	PCP	400	63.713	6.745	6.169	1.00	60.91
ATOM	3432	C1*	PCP	400	63.394	5.459	6.680	1.00	54.96
ATOM	3433	N9	PCP	400	64.326	5.101	7.712	1.00	47.26
ATOM	3434	C4	PCP	400	65.017	3.903	7.840	1.00	46.24

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MOTA 3435 PCP N3 400 64.926 2:770 7.062 1.00 41.02 MOTA C2 3436 PCP 400 65.802 1.878 7.531 1.00 40.72 **ATOM** 3437 N1 PCP 400 66.674 1.917 B.558 1.00 37.37 MOTA 3438 C6 PCP 400 66.735 3.028 9.305 1.00 40.23 **ATOM** 3439 **N6** PCP 400 67.573 3.134 10.333 1.00 33.92 **ATOM** C5 3442 PCP 400 65.862 4.091 8.937 1.00 44.12 MOTA 3443 N7 PCP 400 65.674 5.361 9.472 1.00 45.15 **ATOM** 3444 CB PCP 400 64.761 5.894 8.702 1.00 44.83 MOTA 3445 C2* PCP 400 61.986 5.500 7.254 1.00 57.63 MOTA 3446 02* PCP 400 61.454 4.153 7.211 1.00 56.45 **ATOM** 3448 C3 * PCP 400 61.328 6.402 6.245 1.00 61.31 **ATOM** 3449 03 * PCP 400 60.689 5.644 5.206 1.00 64.65 MOTA 3451 PA PCP 401 9.366 9.801 17.743 0.50 74.43 MOTA 3452 Ola PCP 401 9.463 8.736 16.709 0.50 75.37 MOTA 3453 02A PCP 401 10.330 10.926 17.699 0.50 75.86 **ATOM** 3454 05* PCP 401 9.427 9.108 19.186 0.50 67.44 MOTA 3455 PB PCP 401 6.878 10.679 16.547 0.50 82.27 MOTA 3456 OIR PCP 401 6.223 11.982 16.778 0.50 82.91 ATOM 3457 O2B PCP 6.020 401 9.486 16.408 0.50 82.70 MOTA 3458 PCP **03A** 401 7.868 10.423 17.814 0.50 78.30 MOTA 3459 C3B PCP 401 7.790 10.845 15.159 0.50 82.50 **ATOM** 3460 C5* PCP 401 10.184 9.593 20.275 0.50 54.44 **ATOM** 3461 C4* PCP 401 10.228 8.637 21.442 0.50 45.38 **ATOM** 3462 04* PCP 401 9.032 7.855 21.412 0.50 39.40 MOTA 3463 C1* PCP 401 9.397 6.509 21.641 35.00 0.50 ATOM 3464 N9 PCP 401 8.386 5.627 21.044 0.50 27.91 PCP **ATOM** 3465 C4 7.790 401 21.564 4.469 0.50 23.36 MOTA 3466 N3 PCP 401 7.982 3.849 22.732 0.50 22.33 **ATOM** 3467 C2 PCP 401 7.239 2.768 22.838 0.50 20.26 MOTA 3468 N1 PCP 401 6.382 2.251 22.003 0.50 17.29 **ATOM** 3469 C6 PCP 401 6.202 2.877 20.856 0.50 19.35 MOTA 3470 **N6** PCP 401 5.327 2.415 19.975 0.50 16.87 MOTA 3473 C5 PCP 401 6.932 4.038 20.603 0.50 21.72 MOTA 3474 N7 PCP 401 6.983 4.880 19.507 0.50 24.59 ATOM 3475 CB PCP 401 7.847 5.786 19.832 0.50 24.26 MOTA 3476 C2* PCP 401 10.762 6.409 20.931 0.50 39.01 **ATOM** 02* 3477 PCP 401 11.609 5.326 21.412 0.50 43.88 **ATOM** 3479 C3* PCP 401 11.396 7.674 21.373 0.50 42.14 MOTA 3480 03* PCP 401 11.918 7.515 22.681 0.50 44.21 **ATOM** 3482 N SER 461 78.844 26.057 14.057 1.00 43.87 **ATOM** 3484 CA SER 461 79.399 24.884 13.385 1.00 43.50 ATOM 3485 CB SER 461 78.488 23.655 13.616 1.00 39.99 MOTA 3486 C SER 461 79.572 25.181 11.888 1.00 42.14 MOTA 3487 0 SER 461 79.473 24.292 11.038 1.00 40.29 **ATOM** 3488 N GLU 79.883 462 26.441 11.594 1.00 43.19 MOTA 3490 CA GLU 462 80.061 26.951 10.233 1.00 42.77 MOTA 3491 CB GLU 462 80.303 28.446 10.250 1.00 47.75 MOTA 3492 CG GLU 462 79.209 29.301 10.860 1.00 60.57 **ATOM** 3493 CD GLU 462 79.647 30.752 11.061 1.00 67.56 **ATOM** 3494 OE1 GLU 462 80.866 31.016 10.994 1.00 67.47 **ATOM** 3495 OE₂ GLU 462 78.764 31.611 11.296 1.00 72.32 MOTA 3496 C GLU 462 81.207 26.357 9.457 1.00 39.55 ATOM 3497 0 GLU 462 81.051 26.032 8.292 1.00 38.74 MOTA 3498 N TYR 463 82.375 26.299 10.091 1.00 36.47

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ATOM	3500	CA	TYR	463	83.567	25.806	9.420	1.00	34.19
MOTA	3501	CB	TYR	463	84.702	26.828	9.505	1.00	35.55
MOTA	3502	CG	TYR	463	84.393	28.059	8.675	1.00	42.11
MOTA	3503	CD1	TYR	463	84.004	29.264	9.283	1.00	43.15
MOTA	3504	CE1	TYR	463	83.619	30.361	8.513	1.00	42.40
MOTA	3505	CD2	TYR	463	84.395	27.990	7.280	1.00	39.78
ATOM	3506	CE2	TYR	463	84.012	29.078	6.509	1.00	39.04
ATOM	3507	CZ	TYR	463	83.625	30.256	7.129	1.00	39.86
ATOM	3508	ОН	TYR	463	83.260	31.330	6.366	1.00	42.58
ATOM	3510	С	TYR	463	84.055	24.434	9.800	1.00	33.28
ATOM	3511	0	TYR	463	84.739	23.781	9.005	1.00	33.47
ATOM	3512	N	GLU	464	83.695	23.976	10.993	1.00	34.42
ATOM	3514	CA	GLU	464	84.117	22.660	11.444	1.00	36.38
ATOM	3515	CB	GLU	464	85.618	22.663	11.750	1.00	40.90
MOTA	3516	CG	GLU	464	86.041	23.755	12.729	1.00	46.29
ATOM	3517	CD	GLU	464	87.548	23.810	12.943	1.00	51.33
ATOM	3518	OE1	GLU	464	87.970	24.247	14.038	1.00	54.49
ATOM	3519	OE2	GLU	464	88.312	23.430	12.025	1.00	53.18
MOTA	3520	С	GLU	464	83.374	22.224	12.678	1.00	35.64
ATOM	3521	O	GLU	464	83.111	23.052	13.555	1.00	37.40
ATOM	3522	N	LEU	465	82.962	20.955	12.711	1.00	34.21
ATOM	3524	CA	LEU	465	82.267	20.429	13.887	1.00	34.92
ATOM	3525	CB	LEU	465	81.285	19.300	13.542	1.00	31.30
ATOM	3526	CG	LEU	465	80.272	19.381	12.405	1.00	32.22
ATOM	3527	CD1	LEU	465	79.152	18.407	12.720	1.00	21.95
ATOM ATOM	3528	CD2	LEU	465	79.738	20.802	12.212	1.00	29.75
ATOM	3529 3530	C	LEU	465	83.326	19.855	14.814	1.00	36.17
ATOM	3531	N O	LEU PRO	465	84.473	19.621	14.400	1.00	35.80
ATOM	3532	CD	PRO	466 466	82.970	19.629	16.083	1.00	36.20
ATOM	3533	CA	PRO	466	81.722	20.018	16.758	1.00	38.17
ATOM	3534	CB	PRO	466	83.925 83.132	19.072	17.037	1.00	36.06
ATOM	3535	CG	PRO	466	82.185	19.035 20.194	18.333	1.00	35.57
ATOM	3536	C	PRO	466	84.294	17.666	18.171 16.605	1.00	38.67
ATOM	3537	Ō	PRO	466	83.498	16.959	15.979	1.00	37.06
ATOM	3538	N	GLU	467	85.504	17.258	16.936	1.00	34.50 39.97
ATOM	3540	CA	GLU	467	85.951	15.932	16.587	1.00	44.69
ATOM	3541	CB	GLU	467	87.412	15.985	16.151	1.00	50.43
ATOM	3542	CG	GLU	467	87.902	14.695	15.518	1.00	60.27
ATOM	3543	CD	GLU	467	89.321	14.796	14.986	1.00	65.75
ATOM	3544	OE1	GLU	467	90.024	15.804	15.269	1.00	64.40
ATOM	3545	OE2	GLU	467	89.726	13.850	14.275	1.00	71.13
ATOM	3546	С	GLU	467	85.775	15.002	17.783	1.00	43.30
ATOM	3547	0	GLU	467	85.888	15.428	18.936	1.00	43.26
ATOM	3548	N	ASP	468	85.433	13.750	17.504	1.00	43.09
MOTA	3550	CA	ASP	468	85.254	12.739	18.545	1.00	44.15
MOTA	3551	CB	ASP	468	83.785	12.614	18.979	1.00	44.54
ATOM	3552	CG	ASP	468	83.574	11.562	20.072	1.00	41.84
ATOM	3553	OD1	ASP	468	82.405	11.244	20.368	1.00	39.81
MOTA	3554	OD2	ASP	468	84.570	11.057	20.636	1.00	42.92
MOTA	3555	С	ASP	468	85.746	11.422	17.970	1.00	44.66
MOTA	3556	0	ASP	468	84.982	10.663	17.368	1.00	44.56
ATOM	3557	N	PRO	469	87.034	11.126	18.176	1.00	44.56
MOTA	3558	CD	PRO	469	87.953	11.959	18.971	1.00	45.43

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ATOM 3559 CA PRO 469 87.707 9.916 17.707 1.00 43.90 **ATOM** 3560 СВ PRO 469 89.024 9.959 18.476 1.00 45.66 **ATOM** 3561 CG PRO 469 89.300 11.438 18.547 1.00 44.89 MOTA 3562 C PRO 469 86.934 8.627 17.971 1.00 42.60 MOTA 3563 O PRO 469 86.935 7.730 17.139 1.00 41.35 MOTA 3564 N ARG 470 86.229 8.569 19.096 1.00 43.25 MOTA 3566 CA ARG 470 85.460 7.380 19.470 1.00 44.81 **ATOM** 3567 CB ARG 470 84.722 7.612 20.789 1.00 48.36 **ATOM** 3568 CG ARG 470 85.579 8.201 21.889 1.00 53.41 ATOM 3569 CD ARG 470 84.764 8.458 23.138 1.00 55.42 ATOM 3570 NE ARG 470 83.581 9.261 22.861 1.00 58.57 MOTA 3572 CZ ARG 470 82.748 9.712 23.791 1.00 62.24 ATOM 3573 NH1 ARG 470 82.972 9.445 25.077 1.00 64.57 ATOM 3576 NH2 ARG 470 81.670 10.398 23.436 1.00 63.66 **ATOM** 3579 C ARG 18.437 470 84.439 6.924 1.00 43.69 MOTA 3580 0 ARG 470 84.166 5.735 18.313 1.00 45.68 ATOM 3581 N TRP 471 83.879 7.866 17.693 1.00 42.41 **ATOM** 3583 CA TRP 471 82.851 7 534 16.720 1.00 38.92 MOTA 3584 CB TRP 471 81.577 8.268 17.095 1.00 35.80 **ATOM** 3585 CG TRP 471 80.967 7.741 18.335 1.00 37.13 MOTA 3586 CD2 TRP 471 80.158 6.569 18.443 1.00 37.26 ATOM 3587 CE2 TRP 471 79.723 6.483 19.785 1.00 38.20 ATOM 3588 TRP CE3 471 79.748 5.582 17.530 3.00 35.59 **ATOM** 3589 CD1 TRP 471 81.010 8.300 19.584 1.00 36.42 ATOM 3590 NE1 TRP 471 80.260 7.553 20.462 1.00 35.89 ATOM 3592 CZ2 TRP 471 78.896 5.454 26.239 1.00 36.18 ATOM 3593 CZ3 TRP 471 78.934 4.561 17.978 1.00 32.81 MOTA 3594 CH2 TRP 471 78.514 4.505 19.321 1.00 34.82 **ATOM** 3595 C TRP 471 83.175 7.845 15.277 1.00 39.77 MOTA 3596 TRP 0 471 82.478 7.391 14.362 1.00 39.56 MOTA 3597 N GLU 472 84.224 8.628 15.075 1.00 39.37 MOTA 3599 CA GLU 472 84.605 9.043 13.739 1.00 38.42 MOTA 3600 CB GLU 472 85.794 9.994 13.812 1.00 37.11 MOTA 3601 CG GLU 472 85.958 10.849 12.582 1.00 34.11 MOTA 3602 CD GLU 472 12.33B 84.772 11.757 1.00 34.03 MOTA 3603 OE1 GLU 472 12.348 84.260 13.317 1.00 31.87 ATOM 3604 OE2 GLU 472 84.367 11.885 11.163 1.00 32.11 MOTA 3605 C GLU 472 84.910 7.901 12.791 1.00 39.78 MOTA 3606 0 GLU 472 85.656 6.975 13.128 1.00 41.64 MOTA 3607 N LEU 473 84.303 7.958 11.610 1.00 37.71 MOTA 3609 CA LEU 473 84.538 6.957 10.590 1.00 36.94 MOTA 3610 CB LEU 473 83.258 6.196 10.265 1.00 35.38 **ATOM** 3611 CG LEU 473 83.438 5.065 9.236 1.00 37.67 MOTA 3612 CD1 LEU 473 84.070 3.845 9.903 1.00 37.28 ATOM 3613 CD2 LEU 473 82.106 4.687 8.598 1.00 37.87 MOTA 3614 C LEU 473 85.035 7.664 9.330 1.00 39.31 MOTA 3615 0 LEU 473 84.484 8.697 8.938 1.00 40.55 MOTA 3616 N PRO 474 86.140 7.164 8.732 1.00 39.20 MOTA 3617 CD PRO 87.052 474 6.170 9.327 1.00 37.83 MOTA 3618 CA PRO 474 86.735 7.716 7.513 1.00 38.53 MOTA 3619 CB PRO 474 87.914 6.777 7.282 1.00 37.16 MOTA 3620 CG PRO 474 88.355 6.488 8.644 1.00 34.42 MOTA 3621 C PRO 474 85.733 7.607 6.370 1.00 40.25 MOTA 3622 0 PRO 474 85.220 6.523 6.098 1.00 40.70

PCT/US97/14885

ATOM	3623	N	ARG	475	85.492	8.723	5.685	1.00	41.09
ATOM	3625	CA	ARG	475	84.534	8.746	4.590	1.00	42.26
ATOM	3626	CB	ARG	475	84.487	10.132	3.948	1.00	39.19
ATOM	3627	CG	ARG	475	83.957	11.199	4.876	1.00	35.19
ATOM	3628	CD	ARG	475	84.074	12.593	4.301	1.00	30.76
ATOM	3629	NE	ARG	475	83.796	13.567	5.345	1.00	22.86
ATOM	3631	CZ	ARG	475	82.581	13.898	5.748	1.00	21.99
ATOM	3632	NH1	ARG	475	81.529	13.350	5.165	1.00	23.39
ATOM	3635	NH2	ARG	475	82.412	14.662	6.813	1.00	22.55
ATOM	3638	C	ARG	475	84.838	7.692	3.538	1.00	45.38
ATOM	3639	0	ARG	475	83.927	7.182	2.892	1.00	47.15
ATOM	3640	N	ASP	476	86.106	7.319	3.390	1.00	47.13
ATOM	3642	CA	ASP	476	. 86.461	6.325	2.387	1.00	51.33
ATOM	3643	CB	ASP	476	87.973	6.294	2.134	1.00	55.23
ATOM	3644	CG	ASP	476	88.768	5.841	3.340	1.00	61.15
ATOM	3645	OD1	ASP	476	88.863	4.617	3.573	1.00	65.55
ATOM	3646	OD2	ASP	476	89.331	6.713	4.036	1.00	65.78
ATOM	3647	C	ASP	476	85.932 .	4.940	2.746	1.00	52.35
ATOM ATOM	3648	C	ASP	476	85.815	4.063	1.885	1.00	55.49
ATOM	3649 3651	N CA	ARG	477	85.609	4.752	4.021	1.00	50.77
ATOM			ARG	477	85.080	3.482	4.508	1.00	48.65
ATOM	3652 3653	CB	ARG ARG	477	85.612	3.208	5.908	1.00	50.02
ATOM	3654	CD	ARG	477	87.067	2.799	5.881	1.00	55.33
ATOM	3655	NE	ARG	477	87.760	3.030	7.201	1.00	60.38
ATOM	3657	CZ	ARG	477 4 7 7	87.238	2.207	8.285	1.00	64.36
ATOM	3658	NH1	ARG	477	87.748 88.794	2.203	9.513	1.00	69.16
ATOM	3661	NH2	ARG	477	87.190	2.968 1.459	9.814	1.00	70.73
ATOM	3664	C	ARG	477	83.546	3.414	10.159 4.484	1.00 1.00	71.59
ATOM	3665	o	ARG	477	82.957	2.481	5.013	1.00	46.25 46.36
ATOM	3666	N	LEU	478	82.913	4.372	3.815	1.00	42.23
ATOM	3668	CA	LEU	478	81.464	4.418	3.743	1.00	38.89
MOTA	3669	CB	LEU	478	80.938	5.537	4.657	1.00	37.17
MOTA	3670	CG	LEU	478	79.418	5.733	4.678	1.00	34.13
ATOM	3671	CD1	LEU	478	78.777	4.723	5.609	1.00	32.24
ATOM	3672	CD2	LEU	478	79.074	7.133	5.101	1.00	33.15
MOTA	3673	С	LEU	478	81.059	4.697	2.303	1.00	38.34
ATOM	3674	0	LEU	478	81.515	5.671	1.711	1.00	40.88
MOTA	3675	N	VAL	479	80.208	3.850	1.738	1.00	37.34
MOTA	3677	CA	VAL	479	79.763	4.042	0.364	1.00	37.61
ATOM	3678	CB	VAL	479	80.105	2.829	-0.563	1.00	36.57
ATOM	3679	CG1	VAL	479	79.647	3.105	-1.994	1.00	31.59
ATOM	3680	CG2	VAL	479	81.608	2.567	-0.561	1.06	36.11
ATOM	3681	С	VAL	479	78.267	4.277	0.375	1.00	39.24
ATOM	3682	0	VAL	479	77.484	3.358	0.619	1.00	39.16
ATOM	3683	N	LEU	480	77.894	5.528	0.142	1.00	41.32
ATOM	3685	CA	LEU	480	76.505	5.960	0.123	1.00	41.60
ATOM	3686	CB	LEU	480	76.446	7.480	-0.008	1.00	41.31
ATOM	3687	CG	LEU	480	77.129	8.257	1.118	1.00	39.82
ATOM	3688	CD1	LEU	480	76.985	9.737	0.856	1.00	37.96
ATOM	3689	CD2	LEU	480	76.512	7.887	2.458	1.00	37.70
ATOM	3690	C	LEU	480	75.733	5.312	-1.015	1.00	41.85
ATOM	3691	0	LEU	480	76.235	5.224	-2.131	1.00	45.02
ATOM	3692	N	GLY	481	74.501	4.897	-0.727	1.00	40.86

MOTA	3694	CA	GLY	481	73.673	4.247	-1.727	1.00	40.21
ATOM	3695	С	GLY	481	72.270	4.806	-1.873	1.00	39.78
ATOM	3696	0	GLY	481	72.058	6.015	-1.810	1.00	41.68
ATOM	3697	N	LYS	482	71.306	3.914	-2.063	1.00	39.98
ATOM	3699	CA	LYS	482	69.910	4.297	-2.249	1.00	42.13
ATOM	3700	CB	LYS	482	69.061	3.056	-2.566	1.00	42.73
MOTA	3701	C	LYS	482	69.284	5.050	-1.084	1.00	43.13
ATOM	3702	o	LYS	482	69.373	4.625	0.060	1.00	44.49
ATOM	3703	N	PRO	483	68.676	6.204	-1.358		
ATOM	3704	CD	PRO	483	68.708	6.969		1.00	43.22
ATOM	3704	CA	PRO	483			-2.613	1.00	44.40
ATOM	3706	CB			68.044	6.973	-0.290	1.00	45.44
	3705		PRO	483	67.701	8.295	-0.980	1.00	45.01
MOTA		CG	PRO	483	67.573	7.923	-2.414	1.00	43.95
ATOM	3708	С	PRO	483	66.801	6.261	0.232	1.00	47:67
MOTA	3709	0	PRO	483	66.012	5.725	-0.547	1.00	46.76
ATOM	3710	N	LEU	484	66.650	6.242	1.552	1.00	49.68
MOTA	3712	CA	LEU	484	65.514	5.598	2.196	1.00	54.51
ATOM	3713	CB	LEU	484	65.935	5.026	3.555	1.00	52.70
ATOM	3714	CG	LEU	484	67.132	4.066	3.530	1.00	51.83
ATOM	3715	CD1	LEU	484	67.620	3.766	4.933	1.00	50.19
ATOM	3716	CD2	LEU	484	66.755	2.788	2.825	1.00	52.22
ATOM	3717	С	LEU	484	64.317	6.554	2.357	1.00	58.82
ATOM	3718	0	LEU	484	63.158	6.138	2.244	1.00	60.07
MOTA	3719	N	GLY	485	64.599	7.831	2.609	1.00	61.91
MOTA	3721	CA	GLY	485	63.538	8.810	2.778	1.00	65.89
MOTA	3722	С	GLY	485	64.057	10.167	3.227	1.00	69.46
MOTA	3723	O	GLY	485	65.230	10.301	3.597	1.00	70.65
MOTA	3724	N	GLU	486	63.178	: 11.165 ·	3.241	1.00	70.72
MOTA	3726	CA	GLU	486	63.563	12.521	3.624	1.00	71.32
MOTA	3727	CB	GLU	486	64.015	13.298	2.389	1.00	73.69
ATOM	3728	С	GLU	486	62.435	13.269	4.312	1.00	70.93
MOTA	3729	0	GLU	486	61.281	12.846	4.275	1.00	71.58
MOTA	3730	N	GLY	487	62.781	14.404	4.909	1.00	70.10
MOTA	3732	CA	GLY	487	61.798	15.211	5.603	1.00	68.11
MOTA	3733	C	GLY	487	62.218	16.669	5.598	1.00	67.97
ATOM	3734	0	GLY	487	62.938	17.109	4.696	1.00	67.68
MOTA	3735	N	ALA	488	61.780	17.409	6.615	1 00	67.26
ATOM	3737	CA	ALA	488	62.106	18.826	6.737	1.00	66.90
ATOM	3738	CB	ALA	488	61.362	19.428	7.909	1.00	68.72
ATOM	3739	С	ALA	488	63.607	19.004	6.921	1.00	67.08
MOTA	3740	0	ALA	488	64.124	18.867	8.037	1.00	65.97
MOTA	3741	N	PHE	489	64.297	19.248	5.806	1.00	66.76
ATOM	3743	CA	PHE	489	65.754	19.439	5.773	1.00	65.91
ATOM	3744	CB	PHE	489	66.134	20.794	6.379	1.00	66.45
ATOM	3745	C	PHE	489	66.563	18.288	6.414	1.00	63.92
ATOM	3746	0	PHE	489	67.622	18.503	7.031	1.00	63.16
ATOM	3747	N	GLY	490	66.067	17.069	6.209	1.00	
ATOM	3749	CA	GLY	490	66.710	15.878	6.720		59.03
ATOM	3750	C	GLY	490	66.619			1.00	51.12
ATOM	3751	0				14.823	5.638	1.00	48.59
			GLY	490	65.608	14.736	4.938	1.00	45.25
ATOM	3752	N	GLN	491	67.659	14.003	5.525	1.00	48.77
MOTA	3754	CA	GLN	491	67.732	12.951	4.519	1.00	47.40
ATOM	3755	CB	GLN	491	68.529	13.474	3.319	1.00	49.92
ATOM	3756	CG	GLN	491	68.653	12.514	2.155	1.00	56.31

ATOM	3757	CD	GLN	491	69.604	13.020	1.088	1.00	58.79
ATOM	3758	OE1	GLN	491	70.043	14.171	1.130	1.00	59.63
MOTA	3759	NE2	GLN	491	69.929	12.161	0.122	1.00	59.05
MOTA	3762	C	GLN	491	68.407	11.693	5.086	1.00	44.46
MOTA	3763	0	GLN	491	69.396	11.782	5.806	1.00	44.15
ATOM	3764	N	VAL	492	67.867	10.527	4.752	1.00	42.55
MOTA	3766	CA	VAL	492	68.416	9.247	5.205	1.00	39.22
ATOM	3767	CB	VAL	492	67.375	8.458	6.042	1.00	39.40
MOTA	3768	CGl	VAL	492	67.947	7.127	6.524	1.00	40.17
ATOM	3769	CG2	VAL	492	66.922	9.267	7.210	1.00	36.12
ATOM	3770	С	VAL	492	68.746	8.396	3.975	1.00	37.57
MOTA	3771	O	VAL	492	67.888	8.178	3.115	1.00	35.70
ATOM	3772	N	VAL	493	69.990	7.961.	3.845	1.00	36.27
ATOM	3774	CA	VAL	493	70.333	7.127	2.711	1.00	37.61
ATOM	3775	СВ	VAL	493	71.237	7.863	1.643	1.00	37.45
MOTA	3776	CG1	VAL	493	70.836	9.319	1.524	1.00	38.29
ATOM	3777	CG2	VAL	493	72.717	7.713	1.943	1.00	36.53
ATOM	3778	С	VAL	493	70.952	5.806	3.156	1.00	37.54
ATOM	3779	0	VAL	493	71.542	5.711	4.233	1.00	37.32
ATOM	3780	N	LEU	494	70.691	4.763	2.380	1.00	37.67
ATOM	3782	CA	LEU	494	71.236	3.450	2.656	1.00	38.41
ATOM	3783	CB	LEU	494	70.482	2.387	1.851	1.00	39.16
ATOM	3784	CG	LEU	494	70.834	0.908	2.021	1.00	36.43
ATOM	3785	CD1	LEU	494	70.809	0.508	3.479	1.00	34.69
ATOM	3786	CD2	LEU	494	69.840	0.086	1.229	1.00	37.48
MOTA	3787	С	LEU	494	72.683	3.541	2.202	1.00	39.30
MOTA	3788	O	LEU	494	72.976	4.201	1.207	1.00	39.21
ATOM	3789	N	ALA	495	73.584	2.922	2.954	1.00	40.08
MOTA	3791	CA	ALA	495	74.996	2.954	2.619	1.00	41.70
MOTA	3792	CB	ALA	495	75.654	4.162	3.283	1.00	41.63
ATOM	3793	C	ALA	495	75.670	1.669	3.080	1.00	43.92
ATOM	3794	0	ALA	495	75.033	0.818	3.711	1.00	45.20
MOTA	3795	N	GLU	496	76.946	1.515	2.731	1.00	44.21
MOTA	3797	CA	GLU	496	77.712	0.347	3.137	1.00	43.44
ATOM	3798	CB	GLU	496	78.046	-0.538	1.943	1.00	45.87
MOTA	3799	CG	GLU	496	76.816	-1.142	1.301	1.00	53.11
MOTA	3800	CD	GLU	496	77.145	-2.262	0.339	1.00	56.68
ATOM	3801	OE1	GLU	496	76.473	-3.316	0.410	1.00	61.87
MOTA	3802	OE2	GLU	496	78.068	-2.091	-0.482	1.00	58.18
MOTA	3803	С	GLU	496	78.973	0.773	3.860	1.00	40.97
MOTA	3804	0	GLU	496	79.835	1.437	3.302	1.00	40.91
MOTA	3805	N	ALA	497	79.036	0.439	5.136	1.00	42.07
MOTA	3807	CA	ALA	497	80.173	0.786	5.959	1.00	43.69
ATOM	3808	CB	ALA	497	79.709	1.104	7.366	1.00	40.90
ATOM	3809	С	ALA	497	81.160	-0.372	5.962	1.00	46.16
MOTA	3810	0	ALA	497	80.764	-1.525	5.814	1.00	46.90
ATOM	3811	N	ILE	498	82.446	-0.059	6.090	1.00	48.78
MOTA	3813	CA	ILE	498	83.494	-1.068	6.114	1.00	49.59
ATOM	3814	CB	ILE	498	84.395	-0.993	4.858	1.00	49.46
MOTA	3815	CG2	ILE	498	85.524	-2.006	4.954	1.00	51.16
ATOM	3816	CG1	ILE	498	83.577	-1.244	3.591	1.00	48.96
ATOM	3817	CD1	ILE	498	82.924	0.009	2.998	1.00	52.50
ATOM	3818	С	ILE	498	84.352	-0.877	7.355	1.00	51.33
MOTA	3819	0	ILE	498	84.818	0.230	7.641	1.00	50.42

ATOM 3820 N GLY 499 84.506 -1.952 8.119 1.00 53.87 **ATOM** 3822 CA GLY 499 85.314 -1.909 9.324 1.00 58.16 MOTA 3823 С GLY 499 84.759 -1.094 10.483 1.00 62.44 MOTA 3824 0 GLY 499 85.510 -0.400 11.175 1.00 65.17 **ATOM** 3825 N LEU 500 83.454 -1.187 10.729 1.00 62.92 **ATOM** 3827 CA LEU 500 82.839 -0.453 11.822 1.00 61.93 MOTA 3828 CB LEU 500 81.339 -0.752 11.888 1.00 58.77 MOTA 3829 CG LEU 500 80.501 -0.207 10.736 1.00 56.68 MOTA 3830 CD1 LEU 500 79.047 -0.547 10.964 1.00 55.05 MOTA 3831 CD2 LEU 500 80.682 1.298 10.635 1.00 56.30 **MOTA** 3832 С LEU 500 83.501 -0.B20 13.149 1.00 63.28 MOTA 3833 0 LEU 500 83.623 -2.002 13.487 1.00 64.91 MOTA 3834 N PRO 505 87.387 -6.451 10.091 1.00 82.92 **ATOM** 3835 CD PRO 505 88.522 --6.966 10.874 1.00 83.74 3836 **ATOM** CA PRO 505 -5.052 87.618 9.705 1.00 80.73 MOTA 3837 CB PRO 505 89.027 -4.770 10.247 1.00 81.95 **ATOM** 3838 CG PRO 505 89.655 -6.133 10.342 1.00 83.54 MOTA 3839 C PRO 505 87.514 -4.794 8.205 1.00 77.60 MOTA 3640 0 PRO 505 87.445 -3.651 7.761 1.00 77.24 MOTA 3841 N ASN 506 87.488 -5.863 7.424 1.00 75.24 MOTA 3843 CA ASN 506 87.380 -5.727 5.981 1.00 72.92 MOTA 3844 CB ASN 506 88.435 -6.589 5.283 1.00 73.87 MOTA 3845 C ASN 506 85.978 -6.122 5.529 1.00 70.43 MOTA 3846 0 ASN 506 85.719 -6.281 4.340 1.00 70.01 MOTA 3847 N ARG 507 85.075 -6.273 6.491 1.00 68.31 ATOM 3849 CA ARG 507 83.697 -6.647 6.200 1.00 65.59 **ATOM** 3850 CB ARG 507 83.112 -7.429 7.378 1.00 66.34 **ATOM** 3851 С ARG 507 . 82.846 -5.413 5.941 1.00 62.97 **ATOM** 3852 O ARG 507 83.191 -4.313 6.375 1.00 63.16 **ATOM** 3853 N VAL 508 81.740 ~5.599 5.231 1.00 60.02 ATOM 3855 CA 508 VAL 80.840 -4.495 4.947 1.00 58.59 ATOM 3856 CB VAL 508 80.532 ~4.357 3.439 1.00 58.40 MOTA 3857 CG1 VAL 508 81.813 -4.196 2.658 1.00 61.14 MOTA 3858 CG₂ VAL 508 79.751 -5.**5**53 2.93B 1.00 61.01 MOTA 3859 C VAI. 50R 79.537 -4.682 5.707 1.00 57.24 MOTA 3860 VAL 0 508 79.031 -5.803 5.836 1.00 58.42 MOTA 3861 N THR 509 79.020 ~3.579 6.237 1.00 54.22 MOTA CA 3863 THR 509 77.769 -3.572 6.973 1.00 48.99 MOTA 3864 CB THR 509 77.971 -3.100 8.428 1.00 49.59 MOTA 3865 OG1 THR 509 78.932 -3.935 9.082 1.00 51.71 MOTA 3867 CG2 THR 509 76.665 -3.166 9.198 1.00 50.69 MOTA 3868 С THR 509 76.837 -2.606 6.253 1.00 46.51 MOTA 3869 0 THR 509 77.231 -1.503 5.886 1.00 44.91 MOTA 3870 N LYS 510 75.628 -3.059 5.966 1.00 45.65 MOTA 3872 CA LYS 510 74.658 -2.208 5.314 1.00 43.61 MOTA 3873 CB LYS 510 73.598 -3.058 4.632 1.00 45.46 MOTA 3874 CG LYS 510 72.845 -2.306 3.568 1.00 54.00 MOTA 3875 CD LYS 510 73.022 -2.912 2.183 1.00 58.74 MOTA 3876 CE LYS 510 72.194 -4.184 2.007 1.00 59.63 MOTA 3877 NZ LYS 510 72.711 -5.323 2.815 1.00 61.62 ATOM 3881 С LYS 510 74.065 -1.359 6.450 1.00 42.05 MOTA 3882 0 LYS 510 73.566 -1.898 7 439 1.00 41.29 MOTA 3883 N VAL 511 74.185 -0.038 6.333 1.00 40.14 ATOM 3885 VAL CA 511 73.719

0.894

7.359

1.00

35.38

251

MOTA 3886 CB VAL 511 74.932 1.554 8.074 1.00 33.16 MOTA 3887 CG1 VAL 511 75.761 0.501 8.795 1.00 29.24 ATOM 3888 CG2 VAL 511 75.804 2.295 7.054 1.00 30.37 MOTA 3889 C VAL 72.856 6.776 511 2.005 1.00 33.90 MOTA 3890 0 VAL 511 72.722 2.110 5.558 1.00 32.53 **ATOM** 3891 N ALA 512 72.261 2.813 7.655 1.00 31.97 MOTA 3893 CA ALA 512 71.434 3.956 7.248 1.00 31.10 MOTA 3894 CB ALA 512 70.088 3.945 7.952 1.00 27.38 MOTA 3895 30.49 C ALA512 72.225 5.186 7.660 1.00 MOTA 3896 0 ALA 512 72.775 5.235 8.766 1.00 30.10 **ATOM** 3897 N VAL 72.312 513 6.162 6.765 1.00 30.50 MOTA 3899 CA VAL 513 73.064 7.382 7.041 1.00 29.68 MOTA 3900 CB VAL 513 74.204 7.593 6.015 1.00 28.89 74.966 MOTA 3901 CG1 VAL 513 8.856 6.334 1.00 26.30 MOTA 3902 CG2 VAL 513 6.389 5.987 75.134 1.00 26.66 MOTA 3903 C VAL 513 72.171 B.607 7.012 1.00 28.50 MOTA 3904 0 VAL 513 71.536 8.893 5.994 1.00 26.27 ATOM 3905 N LYS 514 72.091 9.282 8.154 1.00 29.18 MOTA 3907 CA LYS 514 71.307 10.508 8.295 1.00 31.52 MOTA 3908 CBLYS 514 70.797 10.659 9.728 1.00 33.52 MOTA 3909 CG LYS 514 69.890 9.540 10.198 1.00 35.67 MOTA 3910 CDLYS 514 69.439 9.831 11.618 1.00 44.89 MOTA 3911 CE LYS 8.909 514 68.313 12.060 1.00 51 12 MOTA 3912 NZ LYS 514 67.029 9.137 1.00 11.307 57.11 ATOM 3916 С LYS 514 72.233 11.681 7.956 1.00 30.75 MOTA 3917 o LYS 514 73.390 11.698 8.379 1.00 30.08 MOTA 3918 N MET 515 71.724 12.651 7.201 1.00 29.45 **ATOM** 3920 CA MET 515 72.511 13.814 6.786 1.00 28.74 ATOM 3921 CBMET 515 73.342 13.466 5.552 1.00 27.72 ATOM 3922 CG MET 515 72.487 13.034 4.378 1.00 31.56 ATOM 3923 SD MET 515 73.442 12.549 2.945 1.90 34.98 ATOM 3924 CE 73.730 MET 515 10.878 3.330 1.00 31.23 **ATOM** 3925 C MET 515 71.585 14.966 6.444 1.00 27.75 MOTA 3926 0 MET 515 70.369 14.794 6.359 1.00 29.07 ATOM 3927 N LEU 516 72.152 16.145 6.247 1.00 28.33 MOTA 3929 CA LEU 516 71.348 17.313 5.912 1.00 31.16 ATOM 3930 CB LEU 516 72.052 18.605 6.339 1.00 28.70 MOTA 3931 CG LEU 516 72.312 18.866 7.826 1.00 28.33 ATOM 3932 CD1 LEU 516 73.098 20.156 7.949 1.00 28.45 MOTA 3933 CD2 LEU 516 71.020 18.959 8.604 1.00 21.64 MOTA 3934 С LEU 516 71.069 17.378 4.421 1.00 33.22 MOTA 3935 О LEU 516 71.762 16.760 3.619 1.00 35.00 ATOM 3936 LYS N 517 70.022 18.100 4.061 1.00 34.69 ATOM 3938 CA LYS 517 69.696 18.286 2.665 1.00 34.20 MOTA 3939 CB LYS 517 68.194 18.475 2.496 1.00 37.45 MOTA 3940 CG LYS 517 67.403 17.264 2.950 1.00 43.71 **ATOM** 3941 CDLYS 517 66.157 17.072 2.126 1.00 51.25 ATOM 3942 CE LYS 517 65.123 18.135 2.419 1.00 58.56 MOTA 3943 NZ LYS 517 64.010 18.049 1.438 1.00 63.12 MOTA 3947 С LYS 517 70.482 19.533 2.259 1.00 33.81 MOTA 3948 0 LYS 517 70.991 20.244 3.130 1.00 33.17 MOTA 3949 N SER 518 70.603 19.788 0.959 1.00 33.42 MOTA 3951 CA SER 518 71.369 20.938 0.472 1.00 33.33 MOTA 3952 CB SER 518 71.550 20.842 -1.042 1.00 33.23

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ATOM	3953	OG	SER	518	70.306	20.624	-1.678	1.00	38.84
ATOM	3955	C	SER	518	70.794	22.298	0.846	1.00	33.23
MOTA	3956	О	SER	518	71.509	23.305	0.865	1.00	34.14
MOTA	3957	N	ASP	519	69.510	22.313	1.178	1.00	32.77
MOTA	3959	CA	ASP	519	68.825	23.541	1.570	1.00	33.26
MOTA	3960	CB	ASP	519	67.401	23.563	0.995	1.00	35.10
ATOM	3961	CG	ASP	519	66.484	22.503	1.617	1.00	38.98
MOTA	3962	OD1	ASP	519	66.958	21.430	2.042	1.00	37.30
ATOM	3963	OD2	ASP	519	65.261	22.754	1.674	1.00	43.65
ATOM	3964	С	ASP	519	68.793	23.747	3.091	1.00	33.05
ATOM	3965	0	ASP	519	68.114	24.648	3.580	1.00	35.19
ATOM	3966	N	ALA	520	69.538	22.931	3.833	1.00	31.38
ATOM	3968	CA	ALA	-520	69.570	23.032	5.293	1.00	29.47
ATOM	3969	CB	ALA	520	70.264	21.830	5.870	1.00	29.74
ATOM	3970	С	ALA	520	70.229	24.301	5.812	1.00	29.83
ATOM	3971	0	ALA	520	71.004	24.952	5.106	1.00	30.23
MOTA	3972	N	THR	521	69.938	24.616	7.071	1.00	31.57
MOTA	3974	CA	THR	521	70.487	25.793	7.742	1.00	34.56
MOTA	3975	СВ	THR	521	69.361	26.736	8.302	1.00	38.37
ATOM	3976	OG1	THR	521	68.670	26.082	9.376	1.00	41.75
ATOM	3978	CG2	THR	521	68.357	27.117	7.209	1.00	38.30
ATOM	3979	c ·	THR	521	71.353	25.363	8.916	1.00	33.22
MOTA	3980	o	THR	521	71.320	24.207	9.327	1.00	32.31
ATOM	3981	N	GLU	522	72.092	26.310	9.479	1.00	34.43
MOTA	3983	CA	GLU	522	72.951	26.042	10.619	1.00	39.53
ATOM	3984	CB	GLU	522	73.634	27.340	11.068	1.00	46.35
ATOM	3985	CG	GLU	522	74.398	27.271	12.402	1.00	58.03
ATOM	3986	CD	GLU	522	75.772	26.603	12.301	1.00	63.14
MOTA	3987	OEl	GLU	522	76.800	27.321	12.404	1.00	61.75
MOTA	3988	OE2	GLU	522	75.824	25.359	12.158	1.00	66.35
ATOM	3989	С	GLU	522	72.130	25.428	11.765	1.00	38.40
ATOM	3990	С	GLU	522	72.642	24.622	12.543	1.00	37.92
MOTA	3991	N	LYS	523	70.853	25.792	11.849	1.00	36.43
ATOM	3993	CA	LYS	523	69.995	25.261	12.893	1.00	36.83
MOTA	3994	CB	LYS	523	68.703	26.065	13.008	1.00	40.88
MOTA	3995	CG	LYS	523	67.793	25.636	14.152	1.00	44.55
ATOM	3996	CD	LYS	523	66.584	24.898	13.607	1.00	52.68
ATOM	3997	CE	LYS	523	65.629	24.483	14.708	1.00	56.04
ATOM	3998	NZ	LYS	523	64.537	23.646	14.123	1.00	58.13
ATOM	4002	С	LYS	523	69.689	23.804	12.601	1.00	35.27
ATOM	4003	0	LYS	523	69.645	22.985	13.513	1.00	36.58
MOTA	4004	N	ASP	524	69.496	23.473	11.326	1.00	32.27
ATOM	4006	CA	ASP	524	69.235	22.089	10.963	1.00	27.18
ATOM	4007	CB	ASP	524	68.952	21.953	9.480	1.00	26.32
MOTA	4008	CG	ASP	524	67.635	22.555	9.089	1.00	25.22
MOTA	4009	OD1	ASP	524	66.662	22.394	9.848	1.00	31.78
ATOM	4010	OD2	ASP	524	67.568	23.190	8.028	1.00	24.00
ATOM	4011	С	ASP	524	70.445	21.268	11.342	1.00	26.83
ATOM	4012	0	ASP	524	70.312	20.165	11.851	1.00	28.65
MOTA	4013	N	LEU	525	71.633	21.827	11.129	1.00	28.69
ATOM	4015	CA	LEU	525	72.872	21.148	11.473	1.00	26.96
ATOM	4016	CB	LEU	525	74.077	21.981	11.049	1.00	22.80
ATOM	4017	CG	LEU	525	75.445	21.355	11.341	1.00	22.32
ATOM	4018	CD1	LEU	525	75.522	19.883	10.858	1.00	18.89

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ATOM 4019 CD2 LEU 525 76.504 22.212 10.704 1.00 17.44 **ATOM** 4020 C LEU 72.886 20.926 525 12.980 1.00 28.00 MOTA 4021 0 LEU 73.160 19.816 525 13.462 1.00 28.82 MOTA 4022 N SER 72.567 21.992 13.707 526 1.00 27.98 MOTA 4024 CA SER 526 72.496 21.994 15.168 1.00 30.78 MOTA 4025 CB SER 71.939 23.345 526 15.627 1.00 33.18 **ATOM** 4026 OG SER 526 71.624 23.347 17.009 1.00 42.73 **ATOM** 4028 C SER 71.599 526 20.865 15.704 1.00 30.56 ATOM 4029 O SER 526 71.906 20.206 16.716 1.00 31.92 **MOTA** 4030 N ASP 527 70.484 20.665 15.018 1.00 28.19 MOTA 4032 CA ASP 527 69.516 19.651 15.366 1.00 27.41 MOTA 4033 CB ASP 527 68.207 19.932 14.632 1.00 27.63 ATOM 4034 CG ASP 527 6.7.492 21.172 15.149 1.00 27.37 MOTA 4035 OD1 ASP 527 67.870 21.728 16.211 . 1.00 26.70 **ATOM** 4036 OD2 ASP 527 66.525 21.579 14.487 1.00 33.80 **ATOM** 4037 С ASP 527 70.007 18.241 15.063 1.00 27.36 MOTA 4038 C ASP 527 69.722 17.309 15.816 1.00 30.13 **ATOM** 4039 N LEU 528 70.716 18.077 13.952 1.00 25.76 **ATOM** 4041 CA LEU 528 71.245 16.765 13.588 1.00 25.29 ATOM 4042 CB LEU 528 71.777 16.771 12.143 1.00 23.65 ATOM 4043 CG LEU 528 72.283 15.432 11.574 1.00 25.86 MOTA 4044 CD1 LEU 528 71.234 14.341 11.770 1.00 23.35 MOTA 4045 CD2 LEU 528 72.652 15.566 10.102 1.00 17.46 MOTA 4046 c LEU 528 72.351 16.368 14.578 1.00 25.66 MOTA 4047 С LEU 528 72.418 15.210 15.015 1.00 24.02 ATOM 4048 N ILE 529 73.200 17.338 14.934 1.00 26.36 ATOM 4050 CA ILE 529 74.304 17.130 15.886 1.00 26.17 MOTA 4051 CB ILE 529 75.192 16.003 18.381 1.00 22.72 MOTA 4052 CG2 ILE 529 76.250 18.180 17.057 1.00 21.32 ATOM 4053 ILE CG1 529 75.876 18.666 14.685 1.00 20.71 **ATOM** 4054 CD1 ILE 529 76.621 19.965 14.675 1.00 25.60 MOTA 4055 C ILE 529 73.756 16.835 17.283 1.00 29.87 **ATOM** 4056 0 ILE 529 74.253 15.948 17.977 1.00 32.20 **ATOM** 4057 N SER 530 72.741 17.591 17.693 1.00 28.63 MOTA 4059 CA SER 530 72.143 17.381 18.991 1.00 32.21 MOTA 4060 71.031 CB SER 530 18.399 19.231 1.00 37.45 MOTA 4061 OG SER 530 70.065 18.342 18.195 1.00 49.52 **ATOM** 4063 С 530 SER 71.598 15.956 19.075 1.00 30.96 ATOM 4064 0 530 SER 71.728 15.301 20.105 1.00 33.05 MOTA 4065 N GLU **531** 70.996 15.476 17.996 1.00 29.13 **ATOM** 4067 CA GLU 531 70.468 14.117 17.987 1.00 29.84 MOTA 4068 CB GLU 531 69.672 13.847 16.709 1.00 30.29 MOTA 4069 CG GLU 531 69.093 12.445 16.666 1.00 27.39 **ATOM** 4070 CD GLU 531 68.521 12.074 1.00 15.331 31.34 MOTA 4071 OE1 GLU 531 67.929 10.981 15.228 1.00 35.90 MOTA 4072 OE2 GLU 531 68.660 12.860 14.376 1.00 38.37 **ATOM** 4073 C GLU 531 71.600 13.081 18.109 1.00 28.48 **ATOM** 4074 0 GLU 531 71.468 12.094 18.822 1.00 28.17 **ATOM** 4075 N MET 532 72.682 13.281 17.364 1.00 28.12 **ATOM** 4077 CA MET 532 73.832 12.376 17.409 1.00 27.64 **ATOM** 4078 CB MET 532 74.953 12.899 16.499 1.00 26.47 **MOTA** 4079 CG MET 532 76.267 12.125 16.601 1.00 22.25 **ATOM** 4080 SD MET 532 77.406 12.610 15.286 1.00 30.32 **ATOM** 4081 CE MET 532 77.613 14.366 15.661 1.00 20.92

MOTA	4082	С.	MET	532	74.339	12.328	18.832	1.00	27.87
ATOM	4083	0	MET	532	74.640	11.267	19.364	1.00	30.31
MOTA	4084	N	GLU	533	74.439	13.497	19.442	1.00	27.08
ATOM	4086	CA	GLU	533	74.906	13.594	20.802	1.00	28.50
ATOM	4087	CB	GLU	533	75.071	15.064	21.177	1.00	29.09
ATOM	4088	CG	GLU	533	76.216	15.745	20.433	1.00	28.90
ATOM	4089	CD	GLU	533	77.564	15.070	20.661	1.00	31.08
ATOM	4090	OE1	GLU	533	78.001	14.969	21.823	1.00	34.15
MOTA	4091	OE2	GLU	533	78.202	14.643	19.678	1.00	33.60
ATOM	4092	C	GLU	533	73.981	12.850	21.774	1.00	29.91
MOTA	4093	0	GLU	533	74.455	12.093	22.637	1.00	29.73
MOTA	4094	N	MET	534	72.670	13.014	21.588	1.00	29.70
MOTA	4096	CA	MET	534	71.692	12.346	22.444	1.00	27.97
ATOM	4097	CB	MET	534	70.258	12.751	22.082	1.00	28:95
MOTA	4098	CG	MET	534	69.311	12.594	23.278	0.50	29.62 PRT1
MOTA	4099	SD	MET	534	67.538	12.682	22.961	0.50	29.87 PRT1
MOTA	4100	CE	MET	534	67.269	14.452	22.795	0.50	31.07 PRT1
MOTA	4101	C	MET	534	71.855	10.821	22.362	1.00	28.36
MOTA	4102	0	MET	534	71.833	10.143	23.386	1.00	27.02
MOTA	4103	N	MET	535	72.048	10.297	21.151	1.00	26.96
MOTA	4105	CA	MET	535	72.239	8.861	20.947	1.00	26.63
MOTA	4106	CB	MET	535	72.347	8.521	19.456	1.00	24.67
ATOM	4107	CG	MET	535	71.089	8.778	18.659	1.00	23.15
ATOM	4108	SD	MET	535	71.160	8.062	17.011	1.00	24.57
ATOM	4109	CE	MET	535	71.251	9.486	16.023	1.00	24.79
ATOM	4110	С	MET	535	73.498	8.390	21.669	1.00	27.66
ATOM	4111	0	MET	535	73.564	7.259	22.164	1.00	28.83
ATOM	4112	N	LYS	536	74.515	9.246	21.698	1.00	29.13
ATOM	4114	CA	LYS	536	75.757	8.918	22.392	1.00	30.50
ATOM	4115	CB	LYS	536	76.812	9.985	22.131	1.00	29.15
ATOM	4116	CG	LYS	536	77.499	9.883	20.802	1.00	27.71
ATOM	4117	CD	LYS	536	78.377	11.100	20.615	1.00	29.12
ATOM	4118	CE	LYS	536	79.085	11.096	19.279	1.00	26.89
ATOM	4119	NZ	LYS	536	79.688	12.436	19.077	1.00	27.54
ATOM	4123	С	LYS	536	75.480	8.836	23.892	1.00	31.92
MOTA	4124	0	LYS	536	75.921	7.908	24.559	1.00	31.19
ATOM	4125	N	MET	537	74.742	9.814	24.409	1.00	34.02
MOTA	4127	CA	MET	537	74.384	9.881	25.822	1.00	36.35
MOTA	4128	CB	MET	537	73.648	11.197	26.083	1.00	43.33
ATOM	4129	CG	MET	537	73.096	11.376	27.507	1.00	54.60
MOTA	4130	SD	MET	537	71.426	10.674	27.856	1.00	67.38
ATOM	4131	CE	MET	537	71.684	9.813	29.440	1.00	62.03
ATOM	4132	С	MET	537	73.507	8.705	26.253	1.00	34.53
ATOM	4133	0	MET	537	73.744	8.069	27.275	1.00	36.76
MOTA	4134	N	ILE	538	72.496	8.425	25.454	1.00	32.24
MOTA	4136	CA	ILE	538	71.568	7.367	25.757	1.00	29.88
ATOM	4137	CB	ILE	538	70.396	7.384	24.757	1.00	26.98
MOTA	4138	CG2	ILE	538	69.582	6.096	24.842	1.00	27.93
MOTA	4139	CG1	ILE	538	69.527	8.614	25.036	1.00	22.58
MOTA	4140	CD1	ILE	538	68.399	8.787	24.058	1.00	24.58
MOTA	4141	С	ILE	538	72.236	6.006	25.804	1.00	31.83
MOTA	4142	0	ILE	538	71.983	5.227	26.713	1.00	36.32
MOTA	4143	N	GLY	5 39	73.102	5.718	24.848	1.00	32.45
MOTA	4145	CA	GLY	539	73.744	4.422	24.850	1.00	32.13

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MOTA	4146	С	GLY	539	72.974	3.380	24.056	1.00	33.83
ATOM	4147	0	GLY	539	71.876	3.654	23.530	1.00	33.75
ATOM	4148	N	LYS	540	73.539	2.173	24.010	1.00	33.36
ATOM	4150	CA	LYS	540	72.980	1.054	23.256	1.00	37.04
ATOM	4151	CB	LYS	540	74.110	0.181	22.709	1.00	39.21
MOTA	4152	CG	LYS	540	74.865	0.893	21.623	1.00	48.72
MOTA	4153	CD	LYS	540	75.818	0.009	20.850	1.00	56.84
MOTA	4154	CE	LYS	540	76.225	0.693	19.516	1.00	62.14
ATOM	4155	NZ	LYS	540	77.252	-0.102	18.805	1.00	71.02
MOTA	4159	С	LYS	540	71.938	0.162	23.901	1.00	36.51
ATOM	4160	0	LYS	540 .	71.963	-0.096	25.113	1.00	38.52
ATOM	4161	N	HIS	541	71.017	-0.295	23.058	1.00	32.98
ATOM	4163	CA	HIS	541	69.963	-1.230	23.424.	1.00	31.20
MOTA	4164	CB .	HIS	541	68.779	-0.561	24.095	1.00	30.35
ATOM	4165	CG	HIS	541	67.815	-1.540	24.694	1.00	32.56
MOTA	4166	CD2	HIS	541	67.737	-2.058	25.941	1.00	32.45
ATOM	4167	ND1	HIS	541	66.795	-2.124	23.974	1.00	29.22
ATOM	4169	CE1	HIS	541	66.134	-2.965	24.753	1.00	31.56
MOTA	4170	NE2	HIS	541	66.679	-2.932	25.957	1.00	32.22
ATOM	4172	C	HIS	541	69.509	-1.937	22.152	1.00	32.00
MOTA	4173	O	HIS	541	69.409	-1.324	21.095	1.00	32.84
ATOM	4174	N	LYS	542	69.187	-3.222	22.273	1.00	33.61
ATOM	4176	CA	LYS	542	68.786	-4.061	21.154	1.00	31.54
ATOM	4177	CB	LYS	542	68.653	-5.516	21.596	1.00	33.94
MOTA	4178	CG	LYS	542	6.8.322	-6.451	20.437	1.00	42.34
ATOM	4179	CD	LYS	542	68.083	-7.885	20.856	1.00	47.57
ATOM	4180	CE	LYS	542	67.634	-8.726	19.658	1.00	52.70
ATOM	4181	NZ	LYS	542	67.402	-10.146	20.023	1.00	59.51
MOTA	4185	c	LYS	542	67.495	-3.611	20.487	1.00	29.57
MOTA	4186	0	LYS	542	67.268	-3.884	19.305	1.00	27.99
ATOM	4187	N	ASN	543	66.649	-2.931	21.253	1.00	28.32
ATOM	4189	CA	ASN	543	65.378	-2.476	20.714	1.00	28.86
MOTA	4190	CB	ASN	543	64.231	-2.947	21.691	1.00	29.33
MOTA	4191	CG	ASN	543	64.247	-4.452	21.811	1.00	29.64
ATOM	4192	OD1	ASN	543	64.437	-4.926	22.930	1.00	33.86
ATOM	4193	ND2	ASN	543	64.106	-5.206	20.732	1.00	28.02
ATOM	4196	C	ASN	543	65.252	-0.983	20.378	1.00	29.69
ATOM	4197	0	ASN	543	64.159	-0.413	20.457	1.00	30.02
ATOM	4198	N	ILE	544	66.372	-0.357	20.011	1.00	27.35
ATOM	4200	CA	ILE	544	66.382	1.046	19.593	1.00	25.95
MOTA	4201	CB	ILE	544	66.898	2.030	20.706	1.00	25.56
ATOM	4202	CG2	ILE	544	66.148	1.819	22.037	1.00	21.06
ATOM	4203	CG1	ILE	544	68.406	1.901	20.902	1.00	25.61
ATOM	4204	CD1	ILE	544	68.952	2.818	21.976	1.00	25.89
MOTA	4205	С	ILE	544	67.341	1.083	18.399	1.00	25.97
MOTA	4206	0	ILE	544	68.126	0.152	18.227	1.00	25.69
ATOM	4207	N	ILE	545	67.226	2.095	17.537	1.00	27.27
ATOM	4209	CA	ILE	545	68.129	2.243	16.384	1.00	27.02
ATOM	4210	CB	ILE	545	67.541	3.194	15.307	1.00	27.30
ATOM	4211	CG2	ILE	545	68.592	3.553	14.269	1.00	26.52
ATOM	4212	CG1	ILE	545	66.309	2.570	14.638	1.00	22.63
ATOM	4213	CD1	ILE	545	66.605	1.447	13.665	1.00	1 7 .57
ATOM	4214	С	ILE	545	69.383	2.873	16.979	1.00	28.55
ATOM	4215	0	ILE	545	69.346	4.014	17.451	1.00	29.47

ATOM 4216 546 N. ASN 70.482 2.123 16.965 1.00 30.90 MOTA 4218 71.748 CA ASN 546 2.564 17.560 1.00 29.56 **ATOM** 4219 CB ASN 546 72.497 1.365 18.159 1.00 26.32 MOTA 4220 CG ASN 546 71.732 0.695 19.281 1.00 23.81 **ATOM** 4221 OD1 **ASN** 546 71.580 1.252 20.362 1.00 27.34 **ATOM** 4222 ND2 ASN 71.267 546 -0.515 19.039 1.00 23.49 MOTA 4225 С ASN 546 72.700 3.330 16.653 1.00 30.99 **ATOM** 4226 0 ASN 546 72.679 3.169 15.430 1.00 30.98 **ATOM** 4227 N LEU 547 73.543 4.148 17.286 1.00 32.29 **ATOM** 4229 CA LEU 547 74.570 4.948 16.610 1.00 30.93 **ATOM** 4230 CB LEU 547 75.043 6.076 17.542 1.00 25.97 **ATOM** 4231 CG LEU 547 76.075 7.088 17.021 1.00 22.12 4232 ATOM CD1 LEU 547 75.553 15.765 7.815 1.00 22.10 MOTA 4233 CD2 LEU 547 76.415 8.089 18.112 1.00 18.67 ATOM 4234 C LEU 547 75.756 4.039 16.264 1.00 30.70 MOTA 4235 0 LEU 547 76.284 3.361 17.137 1.00 34.46 MOTA 4236 N LEU 76.141 548 3.993 14.992 1.00 30.97 MOTA 4238 CA LEU 548 77.262 3.165 14.562 1.00 30.73 MOTA 4239 CB LEU 76.929 548 2.406 13.281 1.00 29.24 MOTA 4240 CG LEU 548 75.788 1.394 13.371 1.00 28.77 MOTA 4241 CD1 LEU 75.924 548 0.460 12.209 1.00 26.55 MOTA 4242 CD2 LEU 548 75.839 0.616 14.683 1.00 23.48 MOTA 4243 C LEU 78.522 548 3.982 14.347 1.00 33.00 ATOM 4244 0 LEU 548 79.640 3.500 14.558 1.00 35.92 ATOM 4245 N GLY 549 78.351 13.901 5.215 1.00 32.52 ATOM 4247 CA GLY 549 79,503 6.051 13.673 1.00 32.76 MOTA 4248 С GLY 549 79.092 7.411 13.180 1.00 33.72 MOTA 4249 0 GLY 549 77.895 7.707 13.092 1.00 35.01 **ATOM** 4250 N ALA 550 80.089 8.226 12.840 1.00 33.47 MOTA 4252 CA 550 ALA 79.848 9.566 12.337 1.00 30.69 MOTA 4253 CB ALA 550 79.555 10.509 13.497 1.00 28.66 MOTA 4254 550 81.022 C ALA 10.099 11.523 1.00 30.41 **ATOM** 4255 O ALA 550 82.181 9.780 11.808 1.00 25.13 **ATOM** 4256 N CYS 551 80.695 10.817 10.446 1.00 30.29 **ATOM** 4258 CA CYS 551 81.675 11.490 9.584 1.00 28.44 ATOM 4259 CB CYS 551 81.432 11.214 8.096 1.00 27.25 MOTA 4260 SG CYS 551 **B1.639** 9.508 7.566 1.00 28.89 MOTA 4261 C CYS 551 81.337 12.950 9.883 1.00 27.07 MOTA 4262 0 CYS 551 80.293 13.441 9.467 1.00 29.86 MOTA 4263 N THR 552 82.184 13.616 10.658 1.00 25.10 **ATOM** 4265 THR CA 552 81.952 14.997 11.047 1.00 24.37 **ATOM** 4266 CB THR 552 81.959 15.091 12.569 1.00 27.67 **ATOM** 4267 OG1 THR 552 83.271 14.760 13.052 1.00 26.11 MOTA 4269 CG2 THR 552 80.951 14.120 13.164 1.00 30.41 **ATOM** 4270 C THR 552 83.003 15.980 10.557 1.00 24.51 **ATOM** 4271 0 THR 552 82.804 17.194 10.604 1.00 21.56 **ATOM** 4272 N GLN 553 84.151 15.441 10.162 1.00 27.13 **ATOM** 4274 CA GLN 553 85.284 16.243 9.710 1.00 26.64 **ATOM** 4275 CB GLN 553 86.592 15.679 10.283 1.00 25.24 **ATOM** 4276 CG GLN 553 86.641 15.561 11.809 1.00 22.38 MOTA 4277 CD GLN. 553 86.464 16.897 12.515 1.00 24.04 **ATOM** 427R OE1 GLN 553 87.267 17.815 12.344 1.00 31.50 **ATOM** 4279 NE2 GLN 553 85.403 17.017 13.304 1.00 21.59 **ATOM** 4282 С GLN 553 85.384 16.276 8.206 1.00 28.02

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ATOM	4283	0	GLN	553	85.069	15.293	7.537	1.00	30.20
ATOM	4284	N	ASP	554	85.794	17.430	7.695	1.00	28.08
ATOM	4286	CA	ASP	554	86.000	17.652	6.263	1.00	30.14
MOTA	4287	CB	ASP	554	87.330	17.034	5.833	1.00	29.82
MOTA	4288	CG	ASP	554	88.451	17.470	6.707	1.00	31.79
ATOM	4289	OD1	ASP	554	88.699	18.666	6.767	1.00	36.45
MOTA	4290	OD2	ASP	554	89.066	16.623	7.364	1.00	33.06
ATOM	4291	C	ASP	554	84.895	17.217	5.317	1.00	29.52
MOTA	4292	0	ASP	554	85.128	16.411	4.424	1.00	33.67
ATOM	4293	N	GLY	555	83.709	17.793	5.488	1.00	29.02
MOTA	4295	CA	GLY	555	82.586	17.476	4.621	1.00	26.05
MOTA	4296	С	GLY	555	81.286	17.447	5.405	1.00	23.80
ATOM	4297	0	GLY	555	81.269	17.751	6.597	1.00	24.09
ATOM	4298	N	PRO	556	80.175	17.117	4.740	1.00	23.29
ATOM	4299	CD	PRO	556	80.094	16.804	3.304	1.00	18.93
ATOM	4300	CA	PRO	556	78.860	17.045	5.378	1.00	23.45
MOTA	4301	CB	PRO	556	77.943	16.643	4.226	1.00	22.35
ATOM	4302	CG	PRO	556	78.889	15.931	3.261	1.00	24.94
ATOM	4303	С	PRO	556	78.806	16.019	6.503	1.00	26.66
ATOM	4304	0	PRO	556	79.488	14.984	6.464	1.00	27.76
ATOM	4305	N	LEU	557	78.006	16.324	7.522	1.00	29.14
ATOM	4307	CA	LEU	5 57	77.842	15.440	8.676	1.00	30.83
ATOM	4308	CB	LEU	557	77.173	16.181	9.842	1.00	28.40
MOTA	4309	CG	LEU	557	76.775	15.393	11.097	1.00	22.93
ATOM	4310	CD1	LEU	557	77.989	14.897	11.835	1.00	23.02
ATOM	4311	CD2	LEU	557	75.970	16.285	11.984	1.00	23.53
ATOM	4312	c	LEU	557	77.028	14.200	8 321	1.00	31.04
ATOM	4313	O	LEU	557	75.968	14.293	7.634	1.00	31.89
MOTA	4314	N	TYR	558	77.552	13.041	8.700	1.00	29.88
ATOM	4316	CA	TYR	558	76.891	11.773	8.460	1.00	27.80
ATOM	4317	СВ	TYR	558	77.741	10.978	7.562	1.00	28.04
ATOM	4318	CG	TYR	558	77.895	11.339	6.122	1.00	29.98
ATOM	4319	CD1	TYR	558	78.843	10.751	5.289	1.00	31.81
MOTA	4320	CE1	TYR	558	78.980	11.140	3.956	1.00	32.22
ATOM	4321	CD2	TYR	558	77.086	12.335	5.584	1.00	31.50
ATOM	4322	CE2	TYR	558	77.214	12.729	4.256	1.00	31.57
ATOM	4323	CZ	TYR	558	78.166	12.125	3.449	1.00	32.04
ATOM	4324	OH	TYR	558	78.317	12.511	2.134	1.00	33.34
ATOM	4326	C	TYR	558	76.715	11.099	9.809	1.00	27.34
MOTA	4327	0	TYR	558	77.678	10.937	10.558	1.00	25.80
MOTA	4328	N	VAL	559	75.464	10.798	10.147	1.00	28.06
MOTA	4330	CA	VAL	559	75.118	10.118	11.394	1.00	26.67
ATOM	4331	CB	VAL	559	73.930	10.816	12.129	1.00	26.22
ATOM	4332	CG1	VAL	559	73.590	10.079	13.425	1.00	22.58
ATOM	4333	CG2	VAL	559	74.298	12.278	12.440	1.00	23.09
ATOM	4334	C	VAL	559	74.745	8.715	10.943	1.00	24.32
ATOM	4335	0	VAL	559	73.665	8.464	10.412	1.00	26.37
ATOM	4336	N	ILE	560	75.689	7.815	11.095	1.00	23.63
ATOM	4338	CA	ILE	560	75.514	6.448	10.664	1.00	24.67
ATOM	4339	СВ	ILE	560	76.901	5.859	10.299	1.00	24.62
ATOM	4340	CG2	ILE	560	76.753	4.507	9.646	1.00	30.13
ATOM	4341	CG1	ILE	560	77.627	6.B10	9.326	1.00	21.87
ATOM	4342	CD1	ILE	560	79.114	6.538	9.162	1.00	22.25
MOTA	4343	С	ILE	560	74.814	5.621	11.737	1.00	27.30

ATOM	4344	0	ILE	560	75.306	5.505	12.865	1.00	28.80
ATOM	4345	N	VAL	561	73.641	5.090	11.406	1.00	26.80
ATOM	4347	CA	VAL	561	72.894	4.272	12.352	1.00	26.16
MOTA	4348	CB	VAL	561	71.572	4.953	12.810	1.00	24.10
MOTA	4349	CG1	VAL	561	71.866	6.208	13.599	1.00	24.11
ATOM	4350	CG2	VAL	561	70.676	5.254	11.625	1.00	21.97
ATOM	4351	С	VAL	561	72.572	2.901	11.761	1.00	27.98
ATOM	4352	0	VAL	561	72.853	2.632	10.584	1.00	26.49
MOTA	4353	N	GLU	562	71.998	2.039	12.599	1.00	28.86
ATOM	4355	CA	GLU	562	71.605	0.685	12.219	1.00	28.23
MOTA	4356	CB	GLU	562	71.090	-0.068	13.440	1.00	25.86
ATOM	4357	CG	GLU	562	72.170	-0.392	14.424	1.00	27.04
ATOM	4358	CD	GLU	562	71:641	-0.969	15.714	1.00	28.37
ATOM	4359	OE1	GLU	562	72.389	-1.714	16.372	1.00	3-3.36
ATOM	4360	OE2	GLU	562	70.491	-0.665	16.092	1.00	31.60
ATOM	4361	С	GLU	562	70.529	0.720	11.171	1.00	29.67
ATOM	4362	0	GLU	562	69.581	1.489	11.287	1.00	32.53
MOTA	4363	N	TYR	563	70.666	-0.126	10.162	1.00	30.70
ATOM	4365	ĊА	TYR	563	69.699	-0.209	9.083	1.00	30.65
ATOM	4366	CB	TYR	563	70.419	-0.621	7.801	1.00	30.83
ATOM	4367	CG	TYR	563	69.510	-0.905	6.633	1.00	32.10
MOTA	4368	CD1	TYR	563	68.545	0.018	6.235	1.00	33.24
ATOM	4369	CEl	TYR	563	67.715	~0.227	5.160	1.00	34.65
MOTA	4370	CD2	TYR	563	69.609	-2.098	5.922	1.00	31.04
ATOM	4371	CE2	TYR	563	68.779	-2.353	4.838	1.60	33.12
MOTA	4372	CZ	TYR	563	67.831	-1.413	4.470	1.00	34.22
ATOM:	4373	CH	TYR	563	67.902	-1.650	3.400	1.00	34.76
MOTA	4375	С	TYR	563	68.592	-1.223	9.406	1.00	34.39
ATOM	4376	O	TYR	563	68.855	-2.325	9.884	1.00	34.87
ATOM	4377	N	ALA	564	67.356	-0.861	9.091	1.00	35.49
ATOM	4379	CA	ALA	564	66.212	-1.726	9.324	1.00	35.41
MOTA	4380	СВ	ALA	564	65.213	-1.000	10.210	1.00	35.93
ATOM	4381	C	ALA	564	65.585	-2.056	7.962	1.00	37.19
ATOM	4382	0	ALA	564	64.789	-1.276	7.434	1.00	38.08
ATOM	4383	N	SER	565	65.931	-3.211	7.401	1.00	37.14
MOTA	4385	CA	SER	565	65.433	-3.616	6.080	1.00	36.83
MOTA	4386	CB	SER	565	66.151	-4.881,	5.614	1.00	35.24
ATOM	4387	OG	SER	565	66.105	-5.873	6.619	1.00	34.96
MOTA	4389	С	SER	565	63.932	-3782	5.886	1.00	38.65
MOTA	4390	0	SER	565	63.428	-3.617	4.760	1.00	37.80
ATOM	4391	N	LYS	566	63.212	-4.077	6.964	1.00	38.96
MOTA	4393	CA	LYS	566	61.772	-4.271	6.851	1.00	37.83
ATOM	4394	CB	LYS	566	61.357	-5.495	7.655	1.00	39.07
MOTA	4395	CG	LYS	566	61.954	-6.765	7.078	1.00	43.73
MOTA	4396	CD	LYS	566	61.813	-7.950	7.996	1.00	47.07
ATOM	4397	CE	LYS	566	62.258	-9.216	7.299	1.00	47.77
MOTA	4398	NZ	LYS	566	62.361	-10.326	8.278	1.00	51.48
MOTA	4402	С	LYS	566	60.899	-3.050	7.165	1.00	37.53
MOTA	4403	0	LYS	566	59.702	-3.180	7.442	1.00	38.55
ATOM	4404	N	GLY	567	61.496	-1.866	7.066	1.00	35.23
ATOM	4406	CA	GLY	567	60.788	-0.627	7.305	1.00	33.64
MOTA	4407	С	GLY	567	60.120	-0.485	8.656	1.00	33.24
MOTA	4408	0	GLY	567	60.518	-1.133	9.627	1.00	33.80
ATOM	4409	N	ASN	568	59.120	0.389	8.716	1.00	31.65

MOTA	4411	CA	ASN	568	58.407	0.623	9.952	1.00	33.38
MOTA	4412	CB	ASN	568	57.831	2.055	10.025	1.00	37.10
ATOM	4413	CG	ASN	568	56.624	2.272	9.116	1.00	37.78
ATOM	4414	OD1	ASN	568	55.552	1.708	9.337	1.00	41.15
ATOM	4415	MD2	ASN	568	56.780	3.147	8.124	1.00	35.74
ATOM	4418	С	ASN	568	57.357	-0.435	10.263	1.00	33.33
ATOM	4419	0	ASN	568	56.917	-1.178	9.384	1.00	32.54
ATOM	4420	N	LEU	569	56.971	-0.490	11.532	1.00	33.35
MOTA	4422	CA	LEU	569	56.004	-1.455	12.040	1.00	32.38
ATOM	4423	CB	LEU	569	55.838	-1.263	13.552	1.00	27.50
MOTA	4424	CG	LEU	569	54.954	-2.259	14.291	1.00	26.34
ATOM	4425	CD1	LEU	569	55.452	-3.671	14.007	1.00	24.19
ATOM	4426	CD2	LEU	569	54.968	÷1.951	15.787	1.00	21.44
ATOM	4427	C """	LEU	569	54.641	-1.433	11.355	1, 0,0	33.35
ATOM	4428	0	LEU	569	54.060	-2.484	11.095	1.00	34.99
ATOM	4429	N	ARG	570	54.130	-0.239	11.083	1.00	34.36
ATOM	4431	CA	ARG	570	52.827	-0.091	10.445	1.00	36.82
ATOM	4432	CB	ARG	570	52.548	1.393	10.188	1.00	37.28
ATOM	4433	CG	ARG	570	51.210	1.689	9.539	1.00	43.90
MOTA	4434	CD	ARG	570	51.212	3.099	8.967	1.00	50.39
MOTA	4435	NE	ARG	570	52.273	3.268	7.973	1.00	54.99
MOTA	4437	CZ	ARG	570	53.075	4.328	7.887	1.00	54.96
ATOM	4438	NH1	ARG	570	52.947	5.343	8.735	1.00	54.71
ATOM ATOM	4441	NH2	ARG	570	54.030	4.357	6.966	1.00	56.12
ATOM	4444	C O	ARG	570 570	52.818	-0.877	9.133	1.00	36.53
ATOM	4445 4446	N	ARG GLU	570 571	51.968	-1.737	8.909	1.00	34.68
ATOM	4448	CA	GLU	571	53.830	-0.611	8.320	1.00	37.14
ATOM	4449	CB	GLU	571	53.994	-1.253	7.031	1.00	37.94
ATOM	4450	CG	GLU	571	55.126	-0.558	5.274	1.00	39.71
ATOM	4451	CD	GLU	571	54.834 55.934	0.916 1.665	6.062	1.00	44.69
ATOM	4452	OE1	GLU	571	57.098	1.196	5.346 5.358	1.00	52.22
ATOM	4453	OE2	GLU	571	55.629	2.743	4.777	1.00	54.87 56.37
ATOM	4454	C	GLU	571	54.258	-2.744	7.164	1.00	36.53
MOTA	4455	0	GLU	571	53.692	-3.550	6.426	1.00	36.35
MOTA	4456	N	TYR	572	55.105	-3.105	8.120	1.00	35.77
MOTA	445B	CA	TYR	572	55.456	-4.499	8.371	1.00	36.28
ATOM	4459	СВ	TYR	572	56.446	-4.555	9.534	1.00	30.27
ATOM	4460	CG	TYR	572	56.859	-5.925	10.006	1.00	31.65
ATOM	4461	CD1	TYR	572	57.889	-6.626	9.371	1.00	29.40
ATOM	4462	CE1	TYR	572	58.354	-7.839	9.883	1.00	29.32
ATOM	4463	CD2	TYR	572	56.292	-6.480	11.161	1.00	35.17
ATOM	4464	CE2	TYR	572	56.749	-7.696	11.680	1.00	33.08
ATOM	4465	CZ	TYR	572	57.780	-8.366	11.038	1.00	35.15
MOTA	4466	ОН	TYR	572	58.234	-9.559	11.558	1.00	36.91
ATOM	4468	С	TYR	572	54.189	-5.321	8.672	1.00	37.70
ATOM	4469	0	TYR	572	53.942	-6.369	8.068	1.00	36.82
ATOM	4470	N	LEU	573	53.368	-4.799	9.576	1.00	37.64
MOTA	4472	CA	LEU	573	52.126	-5.442	9.970	1.00	36.03
ATOM	4473	CB	LEU	573	51.497	-4.659	11.122	1.00	36.17
ATOM	4474	CG	LEU	573	52.257	-4.641	12.445	1.00	36.39
ATOM	4475	CD1	LEU	573	51.590	-3.665	13.412	1.00	36.17
ATOM	4476	CD2	LEU	573	52.311	-6.042	13.032	1.00	32.13
ATOM	4477	С	LEU	573	51.117	-5.562	8.822	1.00	36.33

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ATOM 4478 LEU 573 0 50.477 -6.596 8.649 1.00 35.19 ATOM 4479 N GLN 574 50.975 -4.502 8.038 1.00 37.66 ATOM 4481 CA GLN 574 50.024 41.78 -4.514 6.936 1.00 **ATOM** 4482 CB 574 -3.103 GLN 49.798 6.413 1.00 43.82 MOTA 4483 CG GLN 574 48.898 -2.273 7.264 1.00 45.42 MOTA 4484 CD GLN 574 48.871 -0.850 6.801 1.00 49.56 **MOTA** 4485 OE1 GLN 574 49.456 -0.506 5.772 1.00 52.22 MOTA NE₂ 4486 GLN 574 48.207 0.001 7.565 1.00 54.86 MOTA 4489 C GLN 574 50.401 -5.427 5.783 1.00 42.B9 MOTA 4490 0 GLN 574 49.532 -5.898 5.042 1.00 46.15 ATOM 4491 N ALA 575 51.695 -5.646 5.599 1.00 42.39 **ATOM** 4493 CA ALA 575 52.165 -6.516 4.532 1.00 40.19 **ATOM** 4494 CB ALA 575 53.597 -6.165 4.170 1.00 40.68 **ATOM** 4495 C ALA 575 52.088 -7.970 4.971 1.00 40.49 MOTA 4496 0 ALA 575 52.437 -8.867 4.210 1.00 43.34 ATOM 4497 N ARG 576 51.630 -8.197 6.202 1.00 38.76 MOTA 4499 CA ARG 576 51.538 -9.542 6.761 1.00 38.44 MOTA 4500 CB ARG 576 52.600 -9.708 7.846 1.00 34.26 MOTA 4501 CG ARG 53.991 576 -9.609 7.284 1.00 37.16 ATOM 4502 CD ARG 576 55.052 -9.625 8.356 1.00 36.38 ATOM 4503 NE ARG 576 56.384 -9.663 7.760 1.00 36.98 MOTA 4505 CZARG 576 56.897 -8.714 6.983 1.00 38.62 MOTA 4506 NH1 ARG 576 56.204 -7.618 6.689 1.00 41.41 MOTA 4509 NH2 ARG 576 58.112 -8.863 5.491 1.00 37.48 MOTA 4512 C ARG 576 50.165 -9.860 7.321 1.00 40.55 MOTA 4513 O 576 ARG 50.013 -10.746 8.169 1.00 43.20 ATOM 4514 N ARG 577 49.156 ~9.146 6.844 1.00 41.98 ATOM 4516 CA 577 ARG 47.794 -9.372 7.309 1.00 43.12 MOTA 4517 CB 577 ARG 46.896 -8.226 6.951 1.00 44.21 MOTA 4518 CG ARG 577 47.206 -6.910 7.525 1.00 45.21 MOTA 4519 CD ARG 577 46.402 -5.766 6.941 1.00 47.50 MOTA 4520 NE ARG 577 46.172 -4.734 7.948 1.00 47.58 MOTA 4522 CZ ARG 577 45.447 -3.641 7.752 1.00 47.63 **ATOM** 4523 NH1 ARG 577 44.882 -3.421 6.574 1.00 49.05 MOTA 4526 NH2 ARG 577 45.256 -2.789 8.747 1.00 49.88 MOTA 4529 C ARG 577 47.241 -10.715 6.821 1.00 43.10 MOTA 4530 0 ARG 577 47.297 -11.015 5.627 1.00 43.86 **ATOM** 4531 N GLN 594 53.448 -13.666 7.976 1.00 64.97 **ATOM** 4533 CA GLN 594 52.231 -13.872 8.759 1.00 66.30 **ATOM** 4534 CB GLN 594 51.419 -15.042 8.200 1.00 67.44 MOTA -14.116 4535 C GLN 594 52.582 10.224 1.00 66.02 MOTA 4536 0 GLN 594 53.162 -15.145 10.583 1.00 67.47 **ATOM** 4537 N LEU 595 52.218 -13.151 11.058 1.00 62.86 **ATOM** 4539 LEU CA 595 52.499 -13.187 12.480 1.00 59.77 MOTA 4540 CB LEU 595 52.597 -11.751 12.987 1.00 59:35 MOTA 4541 CG LEU 595 53.471 -10.905 12.051 1.00 61.70 **ATOM** 4542 CD1 LEU 595 53.307 -9.427 12.322 1.00 64.61 MOTA 4543 CD2 54.923 LEU 595 -11.324 12.175 1.00 62.38 MOTA 4544 C LEU 595 51.482 -13.985 13.290 1.00 57.49 MOTA 4545 0 LEU 595 50.302 -14.026 12.951 1.00 56.36 **ATOM** 4546 N SER 596 51.969 -14.647 14.33B 1.00 55.62 MOTA 4548 CA SER 596 51.134 -15.447 15.222 1.00 54.72 ATOM 4549 CB SER 596 51.905 -16.669 15.721 1.00 55.13 MOTA 4550 OG SER 596 52.871 -16.309 16.69B 1.00 54.98

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MOTA 4552 -14.597 54.73 C SER 596 50.723 16.415 1.00 ATOM 4553 0 SER 596 51.348 -13.579 16.704 1.00 53.29 **ATOM** 4554 49.704 N SER 597 -15.051 17.137 1.00 55.09 **ATOM** 4556 CA SER 597 49.215 -14.337 18.307 1.00 56.44 **ATOM** 4557 CB SER 597 48.178 -15.185 19.044 1.00 59.14 MOTA 4558 OG SER 597 47.455 -16.009 1.00 18.138 65.57 MOTA 4560 C SER 597 50.387 -14.026 19.238 1.00 55.64 **ATOM** 4561 0 SER 597 50.430 -12.966 19.856 1.00 56.04 MOTA 4562 N LYS 598 51.345 ~14.948 19.315 1.00 54.91 MOTA 4564 CA LYS 598 52.528 -14.773 20.161 1.00 54.25 MOTA 4565 CB LYS 598 53.287 -16.096 1.00 54.23 20.311 MOTA 4566 598 CG LYS 54.236 -16.13821.494 1.00 55.12 MOTA 4567 CD LYS 598 55.009 -17.448 21.523 1.00 59.41 MOTA 4568 CE LYS 598 55.711 -17.679 22.858 1.00 58.10 MOTA 4569 NZ LYS 598 54.750 -17.983 1.00 23.959 56.10 MOTA 4573 C LYS 598 53.439 -13.716 19,536 1.00 52.32 **ATOM** 4574 0 LYS 598 53.986 -12.869 20.249 1.00 52.23 MOTA 4575 N ASP 599 53.573 -13.768 18.208 1.00 47.57 MOTA 4577 CA ASP 599 54.389 -12.818 17.466 1.00 45.47 MOTA 4578 CB ASP 599 54.324 -13.101 15.959 1.00 49.05 **ATOM** 4579 CG ASP 599 55.245 -14.238 15.525 1.00 54.16 **ATOM** 4580 OD1 ASP 599 56.242 -14.503 16.223 1.00 61.34 **ATOM** 4581 OD2 ASP 54.992 599 -14.853 14.471 1.00 55.80 MOTA 4582 C ASP 599 53.933 -11.383 17.721 1.00 43.55 MOTA 4583 0 ASP 599 54.762 -10.491 17.895 1.00 44.34 MOTA 4584 N LEU 600 52.622 -11.160 17.751 1.00 39.73 **ATOM** 4586 LEU CA 600 52.104 -9.821 17.989 1.00 37.64 ATOM 50.597 4587 CB LEU 600 -9.743 17.719 1.00 35.42 MOTA 4588 LEU 600 CG 50.075 -9.951 16.287 1.00 33.95 MOTA 4589 CD1 LEU 600 48.621 -9.552 16.262 1.00 36.59 ATOM 4590 CD2 LEU 600 50.841 -9.139 15.265 1.00 28.40 ATOM 4591 C LEU 600 52.429 -9.347 19.402 1.00 38.24 ATOM 19.590 4592 0 LEU 600 52.817 -8.193 1.00 38.28 MOTA 4593 N VAL 601 52.305 -10.235 20.391 1.00 38.77 MOTA 4595 CA VAL 601 52.610 -9.855 21.772 1.00 38.87 MOTA 4596 VAL CB 601 52.121 -10.906 22.812 1.00 38.03 MOTA 4597 CG1 VAL 601 52.150 -10.30324.223 1.00 36.21 MOTA 4598 CG2 VAL 601 50.710 -11.332 22.504 1.00 39.07 MOTA 4599 C VAL 601 54.123 -9.662 21.887 1.00 38.98 MOTA 4600 0 VAL 601 54.601 -8.757 22.580 1.00 39.93 MOTA 4601 N SER 602 54.861 -10.488 21.155 1.00 37.35 ATOM 4603 CA SER 602 56.311 -10.422 21.126 1.00 37.11 MOTA 4604 CB SER 602 56.853 -11.469 1.00 20.154 39.38 MOTA 4605 OG 602 SER 58.265 -11.413 20.061 1.00 46.76 MOTA 4607 С 602 SER 56.695 -9.020 20.664 1.00 35.43 **ATOM** 4608 0 SER 602 57.493 -8.339 21.315 1.00 35.01 **ATOM** 4609 N CYS 603 56.091 -8.586 19.561 1.00 33.42 MOTA 4611 CA CYS 603 -7.254 56.329 19.015 1.00 32.18 MOTA 4612 CB CYS 603 55.449 -7.035 17.790 1.00 32.38 ATOM 4613 SG CYS 603 55.440 -5.365 17.123 0.50 35.11 PRT1 ATOM 4614 С CYS 603 56.074 -6.167 20.059 1.00 31.20 MOTA 4615 603 0 **CYS** 56.862 -5.234 20.185 1.00 32.44 MOTA 4616 N ALA 604 55.001 -6.321 20.828 1.00 29.74 MOTA 4618 CA ALA 604 54.640 -5.363 21.872 1.00 32.26

ATOM	4619	CB	ALA	604	53.232	-5.675	22.412	1.00	31.75
ATOM	4620	С	ALA	604	55.656	-5.365	23.019	1.00	33.71
MOTA	4621	0	ALA	604	55.933	-4.326	23.621	1.00	33.49
MOTA	4622	N	TYR	605	56.186	-6.544	23.326	1.00	35.56
ATOM	4624	CA	TYR	605	57.176	-6.709	24.388	1.00	35.49
MOTA	4625	CB	TYR	605	57.447	-8.206	24.617	1.00	36.12
ATOM	4626	CG	TYR	605	58.562	-8.495	25.591	1.00	34.75
ATOM	4627	CD1	TYR	605	58.415	-8.237	26.954	1.00	34.30
ATOM	4628	CE1	TYR	605	59.444	-8.499	27.853	1.00	36.26
ATOM	4629	CD2	TYR	605	59.773	-9.021	25.150	1.00	37.39
ATOM	4630	CE2	TYR	605	60.812	-9.288	26.040	1.00	37.81
ATOM	4631	CZ	TYR	605	60.641	-9.027	27.388	1.00	38.34
ATOM	4632	OH	TYR	605	61.662	-9.324	28.265	1.00	42.09
ATOM	4634	С	TYR	605	58.475	-5.972	24.027	1.00	34.98
MOTA	4635	O	TYR	605	58.981	-5.171	24.822	1.00	35.83
MOTA	4636	14	GLN	606	58.996	-6.247	22.828	1.00	33.99
ATOM	4638	CA	GLN	606	60.218	-5.620	22.315	1.00	33.60
MOTA	4639	CB	GLN	606	60.506	-6.111	20.894	1.00	31.37
MOTA	4640	CG	GLN	606	60.858	-7.584	20.786	1.00	32.05
MOTA	4641	CD	GLN	606	61.175	-8.015	19.354	1.00	30.33
ATOM	4642	OE1	GLN	606	62.145	-7.558	18.754	1.00	30.84
MOTA	4643	NE2	GLN	606	60.353	-8.895	18.810	1.00	33.75
MOTA	4646	C	GLN	606	60.123	-4.079	22.321	1.00	34.86
ATOM	4647	O	GLN	606	61.070	-3.390	22.702	1.00	37.54
ATOM	4648	N	VAL	607	58.975	-3.555	21.904	1.60	32.89
MOTA	4650	CA	VAL	607	58.748	-2.114	21.983	1.00	30.80
MOTA	4651	CB	VAL	607	57.426	-1.777	21.120	1.00	28.82
ATOM	4652	CG1	VAL	607	57.121	-0.299	21.191	1.00	25.36
ATOM	4653	CG2	VAL	607	57.541	-2.204	19.661	1.00	23.37
ATOM	4654	C.	VAL	607	58.747	-1.532	23.312	1 00	30.48
ATOM	4655	O	VAL	607	59.359	-0.485	23.563	1.00	29.42
ATOM	4656	N	ALA	608	58.106	-2.225	24.255	1.00	30.07
MOTA	4658	CA	ALA	608	58.064	-1.761	25.646	1.00	30.14
MOTA	4659	CB	ALA	608	57.027	-2.548	26.452	1.00	28.49
MOTA	4660	C	ALA	608	59.455	-1.849	26.305	1.00	31.25
MOTA	4661	0	ALA	608	59.791	-1.054	27.198	1.00	28.90
ATOM	4662	N	ARG	609	60.257	-2.819	25.870	1.00	31.61
ATOM	4664	CA	ARG	609	61.608	-2.979	26.393	1.00	31.99
MOTA	4665	CB	ARG	609	62.253	-4.245	25.856	1.00	34.93
ATOM	4666	CG	ARG	609	61.606	-5.507	26.317	1.00	40.82
ATOM	4667	CD	ARG	609	62.633	-6.606	26.397	1.00	42.68
MOTA	4668	NE	ARG	609	63.275	-6.621	27.705	1.00	43.85
ATOM	4670	CZ	ARG	609	64.332	-7.364	28.019	1.00	44.73
MOTA	4671	NH1	ARG	609	64.889	-8.162	27.108	1.00	41.40
MOTA	4674	NH2	ARG	609	64.803	-7.341	29.260	1.00	44.85
MOTA	4677	C	ARG	609	62.459	-1.796	25.966	1.00	33.70
ATOM	4678	0	ARG	609	63.130	-1.174	26.793	1.00	35.94
ATOM	4679	N	GLY	610	62.459	-1.511	24.663	1.00	31.22
MOTA	4681	CA	GLY	610	63.232	-0.391	24.157	1.00	27.21
ATOM	4682	C	GLY	610	62.819	0.875	24.865	1.00	25.81
MOTA	4683	0	GLY	610	63.665	1.652	25.300	1.00	26.21
ATOM	4684	N	MET	611	61.511	1.056	25.015	1.00	27.12
ATOM	4686	CA	MET	611	60.969	2.222	25.695	1.00	28.82
ATOM	4687	CB	MET	611	59.457	2.288	25.524	1.00	29.29

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MOTA 4688 CG MET 611 59.004 2.706 24.135 1.00 31.07 MOTA 4689 SD MET 611 59.732 4.286 23.617 1.00 28.38 MOTA 4690 CE MET 611 59.155 5.431 24.922 1.00 28.34 MOTA 4691 C MET 61.341 2.261 27.178 1.00 611 30.34 MOTA 4692 0 MET 611 61.596 3.334 27.730 1.00 31.73 GLU **ATOM** 4693 N 612 61.347 1.109 27.837 1.00 32.72 **ATOM** 4695 CA GLU 612 61.723 1.057 29.253 1.00 35.46 **ATOM** 4696 CB GLU 612 61.603 -0.370 29.792 1.00 34.70 62.029 MOTA 4697 CG GLU 612 -0.516 31.237 1.00 32.31 **ATOM** 4698 CD GLU 612 62.135 1:968 31.688 1.00 33.14 GLU ATOM 4699 OE1 612 62.546 -2.834 30.883 1.00 30.79 **ATOM** 4700 GLU OE2 612 61.826 -2.240 32.867 1.00 36.13 MOTA 4701 C GLU 612 . 63.178 1.544 29.353 1.00 36.43 ATOM 4702 0 GLU 612 63.534 2.319 30.261 1.00 35.38 **ATOM** 4703 TYR 1.107 N 613 63.999 28.391 1.00 35.47 **ATOM** 4705 CA TYR 613 65.403 1.507 28.334 1.00 33.16 MOTA 4706 CB TYR 613 66.156 0.743 27.241 1.00 31.33 MOTA 4707 CG TYR 613 67.612 1.146 27.132 1.00 33.03 MOTA 4708 CD1 TYR 613 68.584 0.544 27.931 1.00 36.69 MOTA 4709 CE1 TYR 613 69.930 0.927 27.851 1.00 36.82 MOTA 4710 CD2 TYR 613 68.021 2.148 26.247 1.00 33.49 MOTA 4711 CE₂ TYR 69.352 2.540 613 26.157 1.00 34.73 MOTA 70.307 4712 CZ TYR 613 1.927 26.963 1.00 37.07 MOTA 4713 OH TYR 613 71.632 2.318 26.896 1.00 36.77 ATOM 4715 TYR 65.539 3.005 C 613 28.088 1.00 31.82 ATOM 4716 613 28.814 С TYR 66.256 3.682 1.00 34.75 MOTA 4717 LEU 614 3.536 N 64.836 27.090 1.00 28.44 **ATOM** 4719 CA LEU 614 64.931 4.956 26.793 1.00 25.67 ATOM 4720 CB LEU 614 64.089 5.319 25.569 1.00 24.75 MOTA 4721 CC LEU 614 64.545 4.778 24.208 1.00 23.73 MOTA 4722 CD1 LEU 5.257 614 63.594 23.125 1.00 20.54 MOTA LEU 4723 CD2 614 65.983 5.213 23.894 1.00 23,21 MOTA 4724 C LEU 614 64.499 5.761 28.001 1.00 28.30 MOTA 4725 LEU 0 614 65.110 6.770 28.345 1.00 27.09 **ATOM** 4726 ALA N 615 63.470 5.272 28.683 1.00 32.73 MOTA 4728 CA ALA 615 62.955 5.945 29.871 1.00 34.10 MOTA 4729 CB ALA 615 61.625 5.314 30.314 1.00 33.68 MOTA 4730 C ALA 615 63.986 5.913 31.007 1.00 33.84 MOTA 4731 ALA 615 0 64.112 6.885 31.753 1.00 34.95 **ATOM** SER 4732 N 616 64.722 4.809 31.134 1.00 32.69 MOTA 4734 CA SER 616 4.703 1.00 65.738 32.175 33.50 MOTA 4735 CB SER 616 66.287 32.285 3.277 1.00 28.27 MOTA 4736 OG SER 616 67.076 2.935 31.165 1.00 25.54 **ATOM** 4738 C SER 616 66.870 5.678 31.865 1.00 35.43 **ATOM** 4739 О SER 616 67.637 6.061 32.755 1.00 37.32 ATOM 4740 N LYS 617 66.971 6.060 30.592 1.00 34.80 MOTA 4742 CA LYS 617 67.975 7.010 30.143 1.00 33.01 **ATOM** 4743 CB LYS 617 68.508 6.620 28.776 1.00 33.18 MOTA 4744 CG LYS 617 69.224 5.302 28.797 1.00 35.64 MOTA 4745 CD LYS 617 70.423 5.380 29.710 1.00 40.31 **ATOM** 4746 CE LYS 617 71.075 4.025 29.863 1.00 43.03 MOTA 4747 NZ LYS 617 72.426 4.152 30.449 1.00 45.54 ATOM 4751 C LYS 617 67.360 8.397 30.102 1.00 32.87 MOTA 4752 0 LYS 617 67.892 9.308 29.470 1.00 34.06

ATOM	4753	N	LYS	618	66.221	8.542	30.772	1.00	33.53
ATOM	4755	CA	LYS	618	65.500	9.808	30.872	1.00	33.28
MOTA	4756	CB	LYS	618	66.384	10.842	31.558	1.00	37.22
ATOM	4757	CG	LYS	618	66.968	10.367	32.869	1.00	43.11
ATOM	4758	CD	LYS	618	65.927	10.278	33.957	1.00	49.82
ATOM	4759	CE	LYS	618	66.520	9.636	35.199	1.00	55.20
MOTA	4760	NZ	LYS	618	65.669	9.853	36.415	1.00	61.31
ATOM	4764	C	LYS	618	65.012	10.359	29.542	1.00	31.57
ATOM	4765	0	LYS	618	64.651	11.530	29.455	1.00	31.10
ATOM	4766	N	CYS	619	64.953	9.506	28.524	1.00	
ATOM	4768	CA	CYS	619	64.519	9.922	27.196		31.04
ATOM	4769	СВ	CYS	619	65.213	9.065	26.125	1.00	29.21
ATOM	4770	SG	CYS	619	64.782	9.400	24.392		28.55
	4771		CYS	619	62.999	9.849	27.051	1.00	26.31
ATOM	4772	o	CYS	619	62.376	8.827	27.364	1.00	30:91
ATOM	4773	N	ILE	620	62.411	10.967	26.632	1.00	31.18
ATOM	4775	CA	ILE	620	60.981	11.073		1.00	29.48
ATOM	4776	CB	ILE	620	60.402	12.344	26.416	1.00	29.34
ATOM	4777	CG2	ILE	620	58.944		27.060	1.00	28.12
ATOM	4778	CG1	ILE	620	60.521	12.535	26.645	1.00	28.76
ATOM	4779	CD1	ILE	620		12.267	28.581	1.00	28.36
ATOM	4780	C	ILE	620	60.062 60.852	13.522	29.270	1.00	25.55
ATOM	4781	0	ILE	620		11.188	24.908	1.00	30.97
ATOM	4782	N	HIS	621	61.254 60.307	12.193 10.147	24.336	1.00	33.88
ATOM	4784	CA	HIS	621	60.148			1.00	31.55
ATOM	4785	CB	HIS	621	59.721	10.080	22.831	1.00	31.85
ATOM	4786	CG	HIS	621	59.913	8.668 8.373	22.425	1.00	28.27
ATOM	4787	CD2	HIS	621	60.60B	7.383	20.979	1.00	24.68
ATOM	4788	ND1	HIS	621	59.354		20.356	1.00	24.39
ATOM	4790	CE1	HIS	621	59.691	9.130	19.973	1.00	25.87
ATOM	4791	NE2	HIS	621	60.444	8.623.		1.00	27.65
ATOM	4793	C	HIS	621	59.187	7.571 11.096	19.007	1.00	25.80
ATOM	4794	o o	HIS	621	59.387	11.539	22.224	1.00	34.38
ATOM	4795	N	ARG	622	58.080	11.339	21.104	1.00	38.74
ATOM	4797	CA	ARG	622	57.093	12.346	22.898	1.00	37.17
ATOM	4798	CB	ARG	622	57.718	13.746	22.425 22.298	1.00	37.27
ATOM	4799	CG	ARG	622	58.261	14.271		1.00	38.63
ATOM	4800	CD	ARG	622	58.661	15.739	23.601	1.00	40.47
ATOM	4801	NE	ARG	622	59.129	16.174	23.530	1.00	44.76
ATOM	4803	CZ	ARG	622	60.299	15.821	24.842 25.375	1.00	52.09
ATOM	4804	NH1	ARG	622	61.132	15.041	24.699	1.00	56.86
ATOM	4807	NH2	ARG	622	60.606	16.167	26.624	1.00	61.20
ATOM	4810	C	ARG	622	56.324	11.994	21.151	1.00	58.19
ATOM	4811	o	ARG	622	55.300				37.23
ATOM	4812	N	ASP	623	56.805	12.614 11.035	20.867	1.00	38.45
ATOM	4814	CA	ASP	623	56.075		20.364	1.00	36.55
ATOM	4815	СВ	ASP			10.652	19.160	1.00	36.52
ATOM	4816	CG	ASP	623	56.581	11.403	17.910	1.00	39.68
ATOM	4817	OD1	ASP	623	55.635 56.037	11.247	16.687	1.00	48.75
ATOM	4818	OD2		623	56.077	11.491	15.538	1.00	49.98
ATOM	4819		ASP	623	54.445	10.879	16.872	1.00	49.65
ATOM	4820	C	ASP	623	56.126	9.143	18.967	1.00	33.37
		0	ASP	623	56.325	8.650	17.864	1.00	31.77
ATOM	4821	N	LEU	624	55.999	8.404	20.059	1.00	30.45
ATOM	4823	CA	LEU	624	56.014	6.954	19.950	1.00	30.77

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MOTA 4824 CB LEU 624 55.983 6.307 21.342 1.00 27.43 **ATOM** 4825 CG LEU 624 55.949 4.778 21.441 1.00 28.69 **ATOM** 4826 LEU CD1 624 57.139 4.132 20.731 1.00 24.75 MOTA 4827 CD2 LEU 624 55.927 4.389 22.894 1.00 27.39 MOTA 4828 LEU C 624 54.803 6.532 19.109 1.00 31.22 MOTA 4829 O LEU 624 53.680 6.952 19.380 1.00 33.44 MOTA 4830 ALA N 625 55.053 5.763 18.054 1.00 28.85 MOTA 4832 CA ALA 625 54.009 5.286 17.159 1.00 26.93 **ATOM** 4833 CB **ALA** 625 53.559 6.400 16.227 1.00 25.03 MOTA 4834 C ALA 625 54.642 4.162 16.356 1.00 28.44 MOTA 4835 0 ALA 625 55.863 4.065 16.317 1.00 31.32 MOTA 4836 N ALA 626 53.828 3.329 15.705 1.00 29.14 MOTA 4838 CA ALA 626 54.344 2.205 14.905 1.00 28.42 MOTA ALA 4839 CB 626 53.192 1.357 14.353 1.00 27.37 **ATOM** 4840 C ALA 626 55.231 2.698 13.771 1.00 26.38 **ATOM** 4841 0 ALA 626 56.195 2.041 13.395 1.00 26.12 **ATOM** 4842 N ARG 627 54.890 3.861 13.230 1.00 27.16 MOTA 4844 ARG CA 627 55.669 4.474 12.158 1.00 28.44 MOTA 4845 ARG CB 627 55.022 5.794 11.733 1.00 28,19 **ATOM** 4846 CG ARG 627 54.889 6.793 12.867 1.00 30.34 ATOM 4847 CD ARG 627 54.456 8.155 12.361 1.00 34.08 **ATOM** 4848 NE ARG 627 54.081 9.024 13.471 1.00 35.58 ATOM 4850 CZARG 627 52.849 9.123 13.950 1.00 35.55 **ATOM** 4851 **ARG** NH1 627 51.860 8.422 13.420 1.00 35.67 **ATOM** 4854 NH2 ARG 627 52.618 9.898 14.993 1.00 40.81 **ATOM** 4857 C ARG 527 57.108 4.733 12.630 1.00 28.06 MOTA 4858 0 ARG 627 58.044 4.737 11.825 1.00 29.80 **MOTA** 4859 N ASN 628 57.272 4.935 13.940 1.00 28.50 MOTA ASN 4861 CA 628 58.582 5.195 14.544 1.00 26.14 MOTA 4862 CB ASN 628 58.494 6.340 15.551 1.00 23.55 MOTA 4863 CG ASN 628 58.319 7.681 14.874 1.00 27.48 MOTA 4864 ASN OD1 628 58.874 7.919 13.800 1.00 34.12 MOTA 4865 ND2 ASN 628 57.543 8.556 15.479 1.00 23.21 MOTA 4868 C ASN 628 59.263 3.965 15.153 1.00 26.76 MOTA 4869 ASN 0 628 60.202 4.078 15.948 1.00 26.90 MOTA 4870 VAL 629 N 58.774 2.794 14.767 1.00 27.02 MOTA 4872 CA VAL 629 59.344 1.523 15.186 1.00 27.81 MOTA 4873 CB VAL 629 58.298 0.622 15.864 1.00 26.83 MOTA 4874 CG1 VAL 629 58.876 20.74 -0.766 16.115 1.00 MOTA 4875 CG2 VAL 629 57.836 1.259 17.165 1.00 22.49 MOTA 4876 С VAL 629 59.781 0.895 13.861 1.00 28.61 ATOM 58.983 4877 0 VAL 629 0.809 12.924 1.00 28.76 **ATOM** 4878 N LEU 61.059 630 0.557 13.746 1.00 30.35 **MOTA** 4880 CA LEU 630 61.576 -0.033 12.514 1.00 32.42 **ATOM** 4881 CB. LEU 630 62.824 0.725 12.040 1.00 32.28 **ATOM** 4882 CG LEU 630 62.697 2.249 11.880 1.00 27.75 MOTA 4883 CD1 LEU 630 64.019 2.860 11.469 1.00 24.71 MOTA 4884 CD2 LEU 630 2.582 61.611 10.872 1.00 27.70 MOTA 4885 C LEU 630 61.895 -1.488 12.799 1.00 32.89 MOTA 4886 0 LEU 630 62.167 -1.838 13.943 1.00 32.32 **ATOM** 4887 N VAL 631 61.831 -2.336 11.774 1.00 34.81 MOTA 4889 CA VAL 631 62.087 -3.772 11.943 1.00 33.87 **ATOM** 4890 VAL 631 CB 60.818 -4.616 11.597 1.00 31.60 MOTA 4891 CG1 VAL 631 60.929 -6.004 12.197 1.00 30.84

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MOTA 4892 CG2 VAL 631 59.545 -3.916 12.089 1.00 25.53 MOTA 4893 C VAL -4.256 631 63.286 11.109 1.00 34.95 **ATOM** 4894 0 VAL 631 63.365 -4.009 9.892 1.00 37.01 **ATOM** 4895 N THR 632 64.215 -4.942 11.770 35.08 1.00 **ATOM** 4897 CA THR 632 65.418 -5.444 11.104 1.00 35.96 **ATOM** 4898 CB THR 632 66.541 -5.711 12.116 1.00 34.29 **ATOM** 4899 OG1 THR 632 66.187 -6.818 12.953 1.00 32.35 MOTA 4901 CG2 THR 632 66.750 -4.488 12.985 1.00 33.42 **ATOM** 4902 С THR 632 65.162 -6.712 10.300 1.00 39.32 MOTA 4903 0 THR 632 64.078 -7.302 10.382 1.00 41.24 MOTA 4904 N GLU 633 66.153 -7.123 9.511 1.00 42.32 ATOM 4906 CA GLU 633 66.030 -8.335 44.34 8.703 1.00 ATOM 4907 CB GLU 633 67.314 -8.609 7.912 1.00 46.06 ATOM 4908 CG GLU -633 ·· 67:205 -9.767 6.898 1.00 49.87 ATOM 4909 CD GLU 633 66.380 -9.445 5.629 1.00 53.04 ATOM 4910 OE1 GLU 633 65.637 -8.430 5.570 1.00 51.31 MOTA 4911 OE2 GLU 633 66.479 -10.226 4.667 1.00 55.48 MOTA 4912 C GLU 633 65.708 9.600 -9.526 1.00 44.58 MOTA 4913 0 GLU 64.974 633 -10.423 9.207 1.00 46.56 MOTA 4914 N ASP 66.201 634 -9.493 10.833 1.00 44.12 **ATOM** 4916 CA ASP 634 65.961 -10.583 11.759 1.00 44.23 MOTA 4917 CB ASP 67.221 634 -10.867 12.580 1.00 50.17 MOTA 4918 CG ASP 634 68.443 -11.181 11.697 1.00 56.79 **ATOM** 4919 ODI **ASP** 634 68.363 -12.113 10.857 1.00 59.62 MOTA 4920 OD2 **ASP** 634 69.482 -10.490 11.837 1.00 58.62 MOTA 4921 C ASP 64.756 634 -10.331 12.644 1.00 43.26 MOTA 4922 0 ASP 634 64.652 -10.879 13.733 1.00 43.58 MOTA 4923 N ASN 635 63.858 -9.475 12.165 1.00 43.97 MOTA 4925 CA ASN 635 62.612 -9.126 12.847 1.00 43.66 MOTA 4926 CB ASN 635 61.698 -10.355 12.930 1.00 46.94 MOTA 4927 CG ASN 635 61.413 -10.958 11.572 1.00 48.19 MOTA 4928 OD1 ASN 635 60.831 -10.314 10.702 1.00 51.42 MOTA 4929 ND2 ASN 635 61.832 -12.198 11.386 1.00 49.44 MOTA 4932 C ASN 635 62.694 -8.463 14.216 1.00 43.03 ATOM 4933 ASN O 635 61.774 -8.596 15.031 1.00 43.03 4934 MOTA N VAL 636 63.763 -7.712 14.467 1.00 42.69 MOTA 4936 CA VAL 636 63.915 -7.034 15.756 1.00 38.30 **ATOM** 4937 CB VAL 636 65.406 -6.861 16.134 1.00 37.92 MOTA 4938 CG1 VAL 636 65.555 -6.040 17.421 1.00 37.14 MOTA 4939 CG2 VAL 636 66.052 -8.226 16.306 1.00 37.55 MOTA 4940 С VAL 636 63.251 -5.673 15.688 1.00 35.75 ATOM 4941 VAL 0 636 63.486 -4.926 14.746 1.00 36.28 MOTA 4942 N MET 637 62.355 -5.396 16.628 1.00 34.73 MOTA 4944 CA MET 637 61.672 -4.103 16.680 1.00 33.22 MOTA 4945 CB MET 637 60.456 -4.152 17.608 1.00 34.83 ATOM 4946 CG MET 637 59.364 -5.148 17.231 1.00 34.41 MOTA 4947 SD MET 637 58.661 -4.926 15.589 1.00 33.19 MOTA 4948 CE MET 637 58.869 -6.584 14.913 1.00 29.73 MOTA 4949 C MET 637 62.677 -3.107 17.250 1.00 33.75 MOTA 4950 0 MET 637 63.281 -3.357 18.308 1.00 31.79 MOTA 4951 N LYS 638 62.839 -1.980 16.558 1.00 31.83 MOTA 4953 CA-LYS 638 63.774 -0.939 16.965 1.00 28.17 MOTA 4954 CB LYS 638 64.986 -0.930 16.038 1.00 24.98 MOTA 4955 CG LYS 638 66.006 -1.967

16.400

1.00

23.17

267

ATOM 4956 .CD LYS 638 67.193 -1.916 15.470 1.00 25.04 **ATOM** 4957 CE LYS 638 68.212 -2.969 15.847 1.00 24.79 **ATOM** 4958 NZ LYS -2.765 **63B** 68.747 17.220 1.00 24.91 **ATOM** 4962 C LYS 638 63.165 0.445 16.986 1.00 26.04 ATOM 4963 0 LYS 638 62.803 0.958 15.936 1.00 24.44 MOTA 4964 N ILE 639 63.052 1.031 18.181 1.00 25.14 MOTA 4966 CA ILE 639 62.508 2.376 18.351 1.00 25.68 **ATOM** 4967 CB ILE 639 62.589 2.863 19.839 1.00 27.40 MOTA 4968 CG2 ILE 639 61.875 4.189 19.984 1.00 18.94 MOTA 4969 CG1 ILE 639 62.019 1.827 20.826 1.00 26.05 ATOM 4970 CD1 ILE 639 60.517 1.667 20.792 1.00 25.07 4971 ATOM C ILE 639 63.387 3.338 17.543 1.00 25.82 ATOM 4972 O ILE 639 64.619 3.283 17.642 1.00 25.76 ATOM 4973 N ALA 640 62.758 4.231 16.783 1.00 25.92 **ATOM** 4975 CA ALA 640 63.477 5.218 15.976 1.00 26.12 ATOM 4976 CB ALA 640 63.222 4.964 14.506 1.00 26.54 **ATOM** 4977 C ALA 640 63.042 6.643 16.344 1.00 26.33 **ATOM** 4978 0 ALA 640 61.996 6.828 16.974 1.00 26.20 MOTA 4979 N ASP 641 63.863 7.637 15.993 1.00 26.59 MOTA 4981 CA ASP 641 63.545 9.052 16.245 1.00 28.09 MOTA 4982 CB ASP 641 62.217 9.443 15.593 1.00 31.43 **ATOM** 4983 ASP CG 641 62.346 9.762 14.107 1.00 36.81 **ATOM** 4984 OD1 ASP 641 63.409 9.478 13.500 1.00 40.24 ATOM 4985 OD2 ASP 641 61.356 10.299 13.548 1.00 40.49 ATOM 4986 C ASP 641 63.455 9.442 17.700 1.00 28.40 ATOM 4987 0 ASP 641 62.825 10.446 18.041 1.90 29.30 **ATOM** 4988 N PHE 642 64.080 8.658 18.564 1.00 30.27 ATOM 4990 CA PHE 642 64.044 8.943 19.992 1.00 30.97 MOTA 4991 PHE CB 642 64.327 7:664 20.787 1.60 24.64 MOTA 4992 CG PHE 642 65.673 7.063 20.505 1.00 20.96 MOTA 4993 CD1 PHE 642 66.812 7.539 21.163 1.00 16.89 **ATOM** 4994 CD2 PHE 642 65.806 6.026 19.576 1.00 16.23 **ATOM** 4995 CE1 PHE 642 68.072 6.990 20.900 1.00 18.35 **ATOM** 4996 CE2 PHE 642 67.051 5.471 19.305 1.00 18.76 **ATOM** 4997 CZPHE 642 68.195 5.954 19.970 1.00 17.91 MOTA 4998 C PHE 642 65.024 10.045 20.414 1.00 34.53 MOTA 4999 O PHE 642 64.990 10.503 21.563 1.00 35.23 MOTA 5000 N GLY 643 65.910 10.433 19.500 1.00 36.40 MOTA 5002 CA GLY 643 66.888 11.455 19.799 1.00 38.28 MOTA 5003 С GLY 643 66.634 12.768 19.093 1.00 41.44 **ATOM** 5004 O GLY 643 67.482 13.652 19.132 1.00 44.10 MOTA 5005 N LEU 644 65.461 12.921 18.484 1.00 45.44 MOTA 5007 CA LEU 644 65.131 14.144 17.748 1.00 49.14 MOTA 5008 CB LEU 644 63.832 13.975 16.969 1.00 46.26 MOTA 5009 CG LEU 644 63.823 12.967 15.836 1.00 42.90 MOTA 5010 CD1 LEU 644 62.527 13.134 15.070 1.00 42.68 **ATOM** 5011 CD2 LEU 644 65.004 13.228 14.934 1.00 45.15 **ATOM** 5012 С LEU 644 65.027 15.396 18.605 1.00 53.90 MOTA 5013 0 LEU 644 64.488 15.356 19.715 1.00 56.54 ATOM 5014 N ALA 645 65.534 16.505 18.068 1.00 57.59 ATOM 5016 CA ALA 645 65.505 17.794 18.759 1.00 60.15 ATOM 5017 CB 645 ALA 66.539 18.741 18.156 1.00 59.55 ATOM 5018 C ALA 645 64.112 18.407 18.667 1.00 61.90 MOTA 5019 0 ALA 645 63.393 18.500 19.663 1.00 63.83

ATOM	5020	N	ASP	652	52.090	22.191	14.865	1.00	89.91
ATOM	5022	CA	ASP	652	50.913	22.199	14.007	1.00	89.75
ATOM	5023	CB	ASP	652	51.314	22.428	12.537	1.00	88.08
MOTA	5024	CG	ASP	652	50.109	22.557	11.607	1.00	87.09
ATOM	5025	OD1	ASP	652	49.028	22.996	12.052	1.00	86.85
ATOM	5026	OD2	ASP	652	50.252	22.222	10.411	1.00	86.69
MOTA	5027	С	ASP	652	50.145	20.890	14.156	1.00	89.98
MOTA	5028	0	ASP	652	50.434	19.899	13.483	1.00	90.19
MOTA	5029	N	TYR	653	49.145	20.905	15.027	1.00	90.26
ATOM	5031	CA	TYR	653	48.318	19.730	15.277	1.00	90.78
ATOM	5032	CB	TYR	653	47.272	20.048	16.344	1.00	91.65
ATOM	5033	CG	TYR	653	47.804	20.185	17.755	1.00	93.43
ATOM	5034	CD1	TYR	653 ·	47.017	20.757	18.752	1.00	94.60
ATOM	5035	CE1	TYR	653	47.477	20.885	20.058	1:00	95.35
MOTA	5036	CD2	TYR	653	49.083	19.738	18.101	1.00	93.46
ATOM	5037	CE2	TYR	653	49.558	19.860	19.406	1.00	94.36
ATOM	5038	CZ	TYR	653	48.748	20.435	20.378	1.00	95.26
ATOM	5039	ОН	TYR	653	49.220	20.554	21.669	1.00	95.00
ATOM	5041	С	TYR	653	47.602	19.231	14.021	1.00	90.47
ATOM	5042	0	TYR	653	47.045	18.131	14.021	1.00	91.33
ATOM	5043	N	TYR	654	47.632	20.031	12.962	1.00	
ATOM	5045	CA	TYR	654	46.954	19.673	11.727	1.00	39.21 89.09
ATOM	5046	CB	TYR	654	46.205	20.893	11.198	1.00	88.23
ATOM	5047	CG	TYR	654		21.499	12.209	1.00	87.65
ATOM	5048	CD1	TYR	654	45.776	22.140	13.343	1.00	86.76
ATOM	5049	CE1	TYR	654	44.929	22.655	14.312	1.00	87.17
MOTA	5050	CD2	TYR	654	43.895	21.396	12.067	1.00	88.61
ATOM	3051	CE2	TYR	654	43.032	21.912	13.033	1.00	89.32
MOTA	5052	CZ	TYR	654	43.557	22.538	14.153	1.00	88.66
MOTA	5053	ОН	TYR	654	42.710	23.034	15.117	1.00	89.35
ATOM	5055	C	TYR	654	47.857	19.080	10.651	1.00	29.49
ATOM	5056	0	TYR	654	47.396	18.772	9.552	1.00	B8.37
ATOM	5057	N	LYS	655	49.139	18.919	10.959	1.00	90.80
ATOM	5059	CA	LYS	655	50.056	18.356	9.982	1.00	93.18
ATOM	5060	CB	LYS	655	51.508	18.713	10.311	1.00	95.66
ATOM	5061	CG	LYS	655	52.504	18.133	9.315	1.00	99.82
ATOM	5062	CD	LYS	655	53.932	18.585	9.562	1.0010	
ATOM	5063	CE	LYS	655	54.898	17.833	8.637	1.0010	
ATOM	5064	NZ	LYS	655	56.325	18.246	8.821	1.0010	
ATOM	5068	С	LYS	655	49.884	16.847	9.935	1.00	93.56
ATOM	5069	0	LYS	655	49.904	16.182	10.972	1.00	93.72
ATOM	5070	N	LYS	656	49.670	16.320	8.735	1.00	94.19
ATOM	5072	CA	LYS	656	49.500	14.886	8.545	1.00	94.84
MOTA	5073	СВ	LYS	656	48.628	14.620	7.320	1.00	94.64
MOTA	5074	CG	LYS	656	47.155	14.874	7.542	1.00	95.54
ATOM	5075	CD	LYS	656	46.402	14.709	6.241	1.00	99.56
ATOM	5076	CE	LYS	656	44.926	14.449	6.473	1.0010	
ATOM	5077	NZ	LYS	656	44.202	14.327	5.173	1.0010	
ATOM	5081	C	LYS	656	50.859	14.225	8.36B		
ATOM	5082	0	LYS	656	51.823	14.878	7.956	1.00	95.18
ATOM	5083	N	GLY	660	48.651	9.665	7.936 5. 78 2	1.00	95.74 58.76
ATOM	5085	CA	GLY	660	47.932	10.910	6.012	1.00	
ATOM	5086	C	GLY	660	47.241	10.910			56.04
ATOM	5087	0	GLY	660			7.364	1.00	53.90
-11017	5007	J	GHI	300	46.183	11.552	7.525	1.00	53.92

MOTA	5088	N	ARG	661	47.838	10.243	8.328	1.00	51.87
MOTA	5090	CA	ARG	661	47.297	10.177	9.679	1.00	48.23
ATOM	5091	CB	ARG	661	47.755	8.891	10.377	1.00	49.74
ATOM	5092	CG	ARG	661	47.506	7.620	9.566	1.00	47.59
ATOM	5093	CD	ARG	661	47.561	6.390	10.446	1.00	51.85
ATOM	5094	NE	ARG	661	47.584	5.155	9.663	1.00	52.94
ATOM	5096	CZ	ARG	661	48.035	3.988	10.117	1.00	52.19
ATOM	5097	NH1	ARG	661	48.503	3.884	11.356	1.00	52.10
ATOM	5100	NH2	ARG	661	48.036	2.926	9.327	1.00	54.43
ATOM	5103	С	ARG	661	47.722	11.401	10.483	1.00	43.67
ATOM	5104	ō	ARG	661	48.658	12.103	10.104	1.00	41.45
ATOM	5105	N	LEU	662	47.019	11.656	11.579	1.00	40.27
ATOM	5107	CA	LEU	662	47.310	12.799	12.437	1.00	37.15
ATOM	5108	СВ	LEU	662	46.021	13.533	12.783	1.00	37.13
MOTA	5109	CG	LEU	662	45.301	14.149	11.588	1.00	
ATOM	5110	CD1	LEU	662	43.852	14.428	11.937	1.00	
ATOM	5111	CD2	LEU	662	46.041	15.407	11.163	1.00	35.38
ATOM	5112	C	LEU	662	47.973	12.330			39.79
ATOM	5113	0	LEU	662	47.327	11.718	13.716	1.00	34.68
ATOM	5114	N	PRO	663	49.260		14.568	1.00	33.33
ATOM	5115	CD	PRO	663	50.086	12.655	13.892	1.00	34.11
ATOM	5116	CA	PRO	663	50.052	13.389 12.281	12.924	1.00	33.67
ATOM	5117	СВ	PRO	663	51.367	13.003	15.068	1.00	33.55
ATOM	5118	CG	PRO	663	51.479	12.966	14.833	1.00	32.99
ATOM	5119	C	PRO	663	49.412		13.328	1.00	36.09
ATOM	5120	0	PRO	663	49.683	12.665 12.036	16.399	1.00	33.55
ATOM	5121	N	VAL	664	48.566		17.426	1.00	34.11
ATOM	5123	CA	VAL	664	47.874	13.697	16.387	1.00	32.63
ATOM	5124	CB	VAL	664		14.092	17.613	1.00	32.24
ATOM	5125	CG1	VAL	664	46.953	15.327	17.396	1.60	33.24
ATOM	5126	CG2	VAL	664	47.779	16.583	17.252	1.00	35.01
ATOM	5127	C	VAL	664	46.089	15.154	16.155	1.00	35.44
ATOM	5128	0	VAL	664	47.072 46.866	12.896 12.760	18.150	1.00	31.08
ATOM	5129	N	LYS	665			19.360	1.00	31.49
ATOM	5131	CA	LYS	665	46.710	11.978	17.255	1.00	29.75
ATOM	.5132				45.956	10.788	17.638	1.00	28.83
	5133	CB CG	LYS	665	45.411	10.083	16.397	1.00	29.52
ATOM	5134	CD	LYS	665	44.242	10.835	15.797	1.00	27.21
ATOM	5135	CE	LYS	665	43.905	10.431	14.397	1.00	27.25
ATOM	5136	NZ	LYS LYS	665 665	42.684	11.228	13.931	1.00	28.63
ATOM	5140	C			42.266	10.902	12.545	1.00	25.33
ATOM	5141	0	LYS	665 665	46.718	9.830	18.537	1.00	29.03
ATOM	5142	N	LYS TRP		46.152	8.869	19.046	1.00	28.37
ATOM	5144			666	47.994	10.123	18.765	1.00	30.40
ATOM	5145	CA	TRP	666	48.825	9.296	19.628	1.00	31.10
MOTA		CB	TRP	666	50.123	8.906	18.917	1.00	29.53
	5146	CG	TRP	666	49.946	7.781	17.966	1.00	27.03
MOTA	5147	CD2	TRP	666	49.407	7.853	16.638	1.00	25.06
ATOM	5148	CE2	TRP	666	49.418	6.546	16.116	1.00	23.83
ATOM	5149	CE3	TRP	666	48.924	8.899	15.835	1.00	26.08
MOTA	5150	CD1	TRP	666	50.257	6.475	18.186	1.00	20.75
ATOM	5151	NE1	TRP	666	49.937	5.729	17.086	1.00	24.92
ATOM	5153	CZ2	TRP	666	48.962	6.245	14.832	1.00	23.95
ATOM	5154	CZ3	TRP	666	48.466	8.604	14.548	1.00	29.09
ATOM	5155	CH2	TRP	666	48.491	7.282	14.060	1.00	29.22

ATOM 5156 С TRP 666 49.174 10.049 20.896 1.00 33.20 MOTA 5157 0 TRP 666 49.701 9.469 21.849 1.00 34.39 **MOTA** 5158 N MET 667 48.862 11.340 20.910 1.00 34.82 MOTA 5160 CA MET 667 49.169 12.175 22.056 1.00 36.31 MOTA 5161 CB MET 667 49.205 13.645 21.651 1.00 40.08 ATOM 5162 CG MET 667 50.475 14.047 20.931 1.00 42.41 MOTA 5163 SD MET 50.555 667 15.818 20.713 1.00 51.31 MOTA 5164 CE MET 667 50.957 15.928 18.949 1.00 45.44 **ATOM** 5165 C MET 667 48.299 12.003 23.287 1.00 37.81 MOTA 5166 MET 0 667 47.081 11.871 23.195 1.00 38.91 MOTA 5167 N ALA 668 48.958 11.964 24.442 1.00 36.47 **ATOM** 5169 CA ALA 668 48.286 11.846 25.718 1.00 37.06 MOTA 5170 CB ALA 668 49.308 11.654 26.835 1.00 35.76 **ATOM** 5171 C. ALA 668 47.548 13.161 25.893 1.00 38.76 -----**ATOM** 5172 ALA 668 0 48.000 14.201 25.414 1.00 38.04 **ATOM** 5173 N PRO 669 46.416 13.142 26.608 1.00 41.60 ATOM 5174 CD PRO 669 45.819 11.981 27.282 1.00 41.64 MOTA 5175 CA PRO 669 45.614 14.347 26.841 1.00 43.25 MOTA 5176 CB PRO 669 44.478 13.827 27.718 1.00 45.08 ATOM 5177 CG PRO 669 44.383 12.368 27.325 1.00 44.04 ATOM 5178 С PRO 669 46.390 15.486 27.526 1.00 44.68 MOTA 5179 O PRO 669 46.304 16.644 27.111 1.00 43.79 MOTA 5180 N GLU 670 47.135 15.164 28.580 1 00 44.29 **ATOM** 5182 CA GLU 670 47.905 16.195 29.266 1.00 45.36 MOTA 5183 CB GLU 670 48.596 15.637 30.509 1.00 46.97 MOTA 5184 CG GLU 670 49.858 14.819 30.243 1.00 50.04 MOTA 5185 CD GLU 670 49.588 13.345 30.070 1.00 51.35 MOTA 5186 OE1 GLU 570 50.512 12.552 30.327 1.00 50.99 **ATOM** 5187 OE2 GLU 670 48.458 12.975. 29.700 1.00 52.70 MOTA 5188 C GLU 670 48.942 16.802 28.320 1.00 45.63 MOTA 5189 49.174 0 GLU 670 18.006 28.340 1.00 44.75 MOTA 5190 N ALA 671 49.546 15.962 27.482 1.00 46.18 MOTA 5192 CA ALA 671 50.555 16.406 26.531 1.00 46.44 MOTA 5193 CB ALA 671 51.218 15.203 25.860 1.00 43.27 MOTA 5194 С ALA 671 49.931 17.313 25.483 1.00 47.85 MOTA 5195 0 671 ALA 50.485 18.355 25.150 1.00 47.61 MOTA 5196 N LEU 672 48.748 16.928 25.018 1.00 51.40 MOTA 5198 CA LEU 672 48.010 17.657 23.990 1.00 54.25 MOTA 5199 CB LEU 672 46.996 16.705 23.346 1.00 55.60 MOTA 5200 CG LEU 46.202 672 17.113 22.105 1.00 58.92 MOTA 5201 CD1 LEU 672 47.114 17.425 20.932 1.00 58.60 **ATOM** 5202 CD2 LEU 672 45.269 15.977 21.753 1.00 60.32 MOTA 5203 С LEU 672 47.315 18.925 24.514 1.00 55.91 MOTA 5204 0 LEU 672 47.289 19.958 23.837 1.00 55.72 **ATOM** 5205 N PHE 673 46.782 18.846 25.730 1.00 57.88 MOTA 5207 CA PHE 673 46.089 19.977 26.342 1.00 60.07 MOTA 5208 CB PHE 673 44.873 19.484 27.127 1.00 57.08 ATOM 5209 CG PHE 673 43.876 18.742 26.290 1.00 56.39 MOTA 5210 CD1 PHE 673 43.191 17.653 26.813 1.00 57.67 MOTA 5211 CD2 PHE 673 43.633 19.116 24.970 1.00 55.36 MOTA 5212 CE1 PHE 673 42.281 16.939 26.036 1.00 57.42 MOTA 5213 CE2 PHE 673 42.724 18.410 24.183 1.00 55.91 MOTA 5214 CZ PHE 673 42.049 17.317 24.720 1.00 56.42 **MOTA** 5215 C PHE 673 46.974 20.854 27.238 1.00 63.00

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MOTA PHE 22.085 27.155 5216 O 673 46.926 1.00 65.31 **ATOM** 20.223 28.081 5217 N **ASP** 674 47.786 1.00 64.08 **ATOM** 5219 20.954 28.999 CA ASP 674 48.656 1.00 64.97 **MOTA** 5220 CB **ASP** 674 48.545 20.375 30.409 1.00 65.13 **ATOM** 5221 CG ASP 674 47.128 20.358 30.923 1.00 67.33 5222 ATOM **ASP** 46.684 OD1 674 19.283 31.372 1.00 66.68 MOTA 5223 QD2 ASP 674 46.462 21.416 30.869 1.00 69.20 674 MOTA 5224 С ASP 50.132 20.971 28.603 1.00 66.38 MOTA 5225 50.984 29.434 0 **ASP** 674 21.304 1.00 68.44 MOTA 5226 N ARG 675 50.441 20.585 27.365 1.00 65.68 **ATOM** 5228 CA ARG 675 51.829 20.550 26.883 1.00 63.71 **ATOM** 5229 CB ARG 675 52.321 21.970 26.576 1.00 63.67 MOTA 5230 CG ARG 675 51.491 22.685 25.531 1.00 67.65 MOTA 5231 CD ARG 675 52.094 24.034 25.146 1.00 73.20 **ATOM** 5232 NE ARG 675 53.382 23.911 24.457 1.00 74.09 MOTA 5234 CZARG 675 54.159 24.939 24.122 1.00 73.41 MOTA 5235 NH1 ARG 675 53.788 26.182 24.408 1.00 72.90 MOTA 5238 NH2 ARG 675 55.324 24.720 23.524 1.00 71.96 MOTA 5241 C ARG 675 52.780 19.864 27.876 1.00 61.41 MOTA 5242 О ARG 675 53.960 20.208 27.966 1.00 62.62 ATOM 5243 N ILE 676 52.248 18.903 28.627 1.00 59.15 ATOM 5245 CA ILE 676 53.016 18.162 29.623 1.00 56.88 MOTA 5246 CB ILE 676 52.175 17.904 30.891 1.00 56.26 MOTA 5247 CG2 ILE 675 52.871 16.904 31.807 1.00 53.11 MOTA 5248 CG1 ILE 51.920 676 19.224 31.614 1.00 57.86 **ATOM** 5249 CD1 ILE 676 51.038 19.096 32.835 1.00 61.05 **MOTA** 5250 C ILE 676 53.494 16.828 29.070 1.00 56.58 ATOM 5251 0 ILE 676 52.727 15.869 28.985 1.00 58.12 **ATOM** 5252 N TYR 677 54.760 16.773 28.680 1.00 54.34 MOTA 5254 TYR 55.340 CA 677 15.556 28.143 1.00 51.14 **ATOM** 5255 CB TYR 677 56.240 15.868 26.954 1.00 52.37 **ATOM** 5256 CG TYR 677 55.488 16.315 25.719 1.00 56.21 MOTA 5257 CD1 TYR 677 55.187 17.660 25.512 1.00 56.78 MOTA 5258 CE1 TYR 677 54.534 18.086 24.353 1.00 57.54 MOTA 5259 CD2 TYR 677 55.113 15.395 24.738 1.00 57.82 MOTA 5260 CE2 TYR 677 54.458 15.809 23.571 1.00 59.32 MOTA 5261 CZ677 59.59 TYR 54.177 17.159 23.385 1.00 MOTA 5262 OH TYR 677 53.557 17.589 22.230 1.00 60.15 MOTA 5264 С TYR 677 56.124 14.854 29.224 1.00 48.64 MOTA 5265 0 TYR 677 57.040 15.430 29.812 1.00 50.45 MOTA 5266 N THR 678 55.733 13.621 29.510 1.00 44.59 MOTA 5268 CA THR 678 56.397 12.834 30.524 1.00 42.21 ATOM 5269 CB THR 678 55.524 12.726 31.791 1.00 43.55 MOTA 5270 OG1 THR 678 12.045 54.302 31.475 1.00 47.42 **ATOM** 5272 CG2 THR 678 55.190 14.105 32.327 1.00 48.74 **MOTA** 5273 C THR 678 56.634 11.432 29.992 1.00 39.94 **ATOM** 5274 0 THR 678 56.207 11.085 28.892 1.00 39.34 MOTA 5275 N 679 HIS 57.312 10.616 30.784 1.00 38.54 MOTA 5277 CA HIS 679 57.532 9.248 30.390 1.00 38.29 ATOM 5278 CB 679 HIS 58.441 8.546 31.391 1.00 39.51 ATOM 5279 CG HIS 679 59.869 8.997 31.331 1.00 43.13 CD2 ATOM 5280 HIS 679 60.630 9.668 32.233 1.00 43.49 **ATOM** 5281 ND1 HIS 679 60.694 8.726 30.263 1.00 43.00 ATOM 5283 CE1 HIS 679 61.903 9.201 30.510 1.00 43.62

ATOM	5284	NE2	HIS	679	61.889	9.778	31.695	1.00	44.68
MOTA	5286	С	HIS	679	56.147	8.599	30.359	1.00	39.42
ATOM	5287	0	HIS	679	55.898	7.667	29.593	1.00	40.00
ATOM	5288	N	GLN	680	55.228	9.156	31.142	1.00	38.96
ATOM	5290	CA	GLN	680	53.867	8.649	31.209	1.00	38.84
ATOM	5291	CB	GLN	680	53.214	9.010	32.543	1.00	40.90
MOTA	5292	CG	GLN	680	53.835	8.278	33.732	1.00	44.42
MOTA	5293	CD	GLN	680	53.677	6.756	33.660	1.00	44.47
ATOM	5294	OE1	GLN	680	52.595	6.225	33.908	1.00	45.52
MOTA	5295	NE2	GLN	680	54.767	6.050	33.348	1.00	42.06
ATOM	5298	C	GLN	680	53.013	9.099	30.036	1.00	38.25
MOTA	5299	O	GLN	680	51.968	8.505	29.758	1.00	39.27
MOTA	5300	N	SER	681	53.427	10.155	29.349	1.00	37.00
ATOM	5302	CA	SER	681	-52.665	10.571	28.182	1.00	38.02
MOTA	5303	CB	SER	681	52.929	12.034	27.813	1.00	40.29
ATOM	5304	OG	SER	681	54.307	12.286	27.620	1.00	47.29
MOTA	5306	С	SER	681	53.066	9.620	27.051	1.00	37.43
ATOM	5307	0	SER	681	52.289	9.366	26.136	1.00	37.86
ATOM	5308	N	ASP	682	54.281	9.077	27.162	1.00	35.23
MOTA	5310	CA	ASP	682	54.800	8.106	26.205	1.00	33.24
MOTA	5311	CB	ASP	682	56284	7.820	26.464	1.00	31.85
ATOM	5312	CG	ASP	682	57.224	8.732	25.677	1.00	34.18
ATOM	5313	OD1	ASP	682	58.445	8.537	25.826	1.00	31.79
ATOM	5314	OD2	ASP	682	56.763	9.620	24.908	1.00	29.15
ATOM	5315	С	ASP	682	54.015	6.810	26.374	1.00	31.52
MOTA	5316	С	ASP	682	53.788	6.087	25.411	1.00	31 93
ATOM	5317	W	VAL	683	53.653	6.499	27.617	1.00	33.14
MOTA	5319	C:A	VAL	683	52.879	5.293	27.935	1.00	32.79
ATOM	5320	CB	VAL	683	52.725	5.095	29.478	1.00	34.55
ATOM	5321	CG1	VAL	683	51.653	4.059	29.790	1.00	32.39
ATOM	5322	CG2	VAL	683	54.050	4.649	30.088	1.00	28.08
ATOM	5323	C	VAL	683	51.506	5.338	27.245	1.00	31.45
ATOM	5324	O	VAL	683	51.008	4.311	26.779	1.00	30.37
ATOM	5325	N	TRP	684	50.919	6.531	27.147	1.00	31.04
ATOM	5327	CA	TRP	684	49.638	6.686	26.464	1.00	31.23
MOTA	5328	CB	TRP	684	49.158	8.137	26.525	1.00	34.14
MOTA	5329	CG	TRP	684	47.913	8.423	25.694	1.00	37.17
ATOM	5330	CD2	TRP	684	46.573	8.593	26.187	1.00	38.61
MOTA	5331	CE2	TRP	684	4 5. 75 5	8.888	25.064	1.00	37.91
MOTA	5332	CE3	TRP	684	45.978	8.528	27.452	1.00	37.63
MOTA	5333	CD1	TRP	684	47.850	8.612	24.337	1.00	37.39
ATOM	5334	NE1	TRP	684	46.560	8.894	23.956	1.00	34.76
ATOM	5336	CZ2	TRP	684	44.380	9.118	25.181	1.00	34.79
ATOM	5337	CZ3	TRP	684	44.611	8.759	27.563	1.00	38.53
MOTA	5338	CH2	TRP	684	43.830	9.048	26.428	1.00	37.59
MOTA	5339	С	TRP	684	49.876	6.294	25.013	1.00	29.99
MOTA	5340	0	TRP	684	49.254	5.356	24.503	1.00	30.82
MOTA	5341	N	SER	685	50.815	6.992	24.380	1.00	28.28
MOTA	5343	CA	SER	685	51.174	6.738	22.986	1.00	27.54
ATOM	5344	CB	SER	685	52.444	7.504	22.631	1.00	26.69
MOTA	5345	OG	SER	685	52.355	8.874	22.986	1.00	32.15
ATOM	5347	C	SER	685	51.39 9	5.249	22.737	1.00	26.41
MOTA	5348	0	SER	685	50.968	4.709	21.713	1.00	29.52
MOTA	5349	N	PHE	686	52.065	4.582	23.676	1.00	26.47

ATOM	5351	CA	PHE	686	52.325	3.151	23.563	1.00	26.35
ATOM	5352	CB	PHE	686	53.167	2.668	24.754	1.00	25.01
MOTA	5353	CG	PHE	686	53.447	1.182	24.742	1.00	27.24
MOTA	5354	CD1	PHE	686	54.187	0.600	23.712	1.00	24.88
MOTA	5355	CD2	PHE	686	52.915	0.351	25.729	1.00	24.99
ATOM	5356	CE1	PHE	686	54.389	-0.783	23.655	1.00	22.77
ATOM	5357	CE2	PHE	686	53.113	-1.036	25.679	1.00	28.39
ATOM	5358	CZ	PHE	686	53.853	-1.601	24.631	1.00	22.71
MOTA	5359	С	PHE	686	50.997	2.366	23.466	1.00	28.82
MOTA	5360	0	PHE	686	50.892	1.398	22.696	1.00	26.41
ATOM	5361	N	GLY	687	49.988	2.797	24.229	1.00	29.65
ATOM	5363	CA	GLY	687	48.692	2.134	24.194	1.00	29.88
ATOM	5364	С	GLY	687	48.099	2.158	22.794	1.00	29.57
ATOM	5365	o	GLY	687	47.560	1.165	22.300	1.00	30.38
ATOM	5366	N	VAL	688	48.222	3.310	22.147	1.00	29.19
MOTA	5368	CA	VAL	688	47.718	3.478	20.795	1.00	25.09
ATOM	5369	CB	VAL	688	47.747	4.956	20.359	1.00	22.52
MOTA	5370	CG1	VAL	688	47.106	5.115	18.985	1.00	21.13
MOTA	5371	CG2	VAL	688	47.001	5.810	21.366	1.00	22.50
ATOM	5372	C	VAL	688	48.574	2.636	19.865	1.00	23.82
ATOM	5373	0	VAL	688	48.080	2.132	18.871	1.00	25.39
ATOM	5374	Ŋ	LEU	689	49.849	2.463	20.208	1.00	24.46
ATOM	5376	CA	LEU	689	50.764	1.655	19.401	1.00	25.68
ATOM	5377	CB	LEU	689	52.222	1.893	19.834	1.00	25.93
MOTA	5378	CG	LEU	689	53.374	1.307	19.004	1.00	25.01
MOTA	5379	CDI	LEU	689	54.655	2.080	19.257	1.00	25.86
MOTA	5380	CD2	LEU	689	53.593	-0.145	19.318	1.00	24.90
ATOM	5381	C	LEU	689	50.374	0.171	19.531	1.00	26.50
ATOM	5382	Ó	LEU	689	50.464	-0.578	18.558	1.00	27.13
MOTA	5383	N	LEU	690	49.927	-0.234	20.724	1.00	27.76
MOTA	5385	CA	LEU	690	49.481	-1.610	20.980	1.00	28.59
MOTA	5386	CB	LEU	690	49.087	-1.800	22.447	1.00	30.38
ATOM	5387	CG	LEU	690	50.121	-2.065	23.545	1.00	29.57
MOTA	5388	CD1	LEU	690	49.435	-1.966	24.907	1.00	27.40
ATOM	5389	CD2	LEU	690	50.744	-3.431	23.360	1.00	28.79
ATOM	5390	C	LEU	690	48.242	-1.849	20.134	1.00	28.77
ATOM	5391	0	LEU	690	48.055	-2.922	19.573	1.00	28.07
MOTA	5392	N	TRP	691	47.383	-0.838	20.075	1.00	29.58
MOTA	5394	CA	TRP	691	46.166	-0.921	19.275	1.00	30.53
MOTA	5395	CB	TRP	691	45.327	0.349	19.451	1.00	28.28
ATOM	5396	CG	TRP	691	43.985	0.300	18.769	1.00	25.86
MOTA	5397	CD2	TRP	691	43.702	0.689	17.421	1.00	23.99
ATOM	5398	CE2	TRP	691	42.321	0.498	17.215	1.00	25.08
ATOM	5399	CE3	TRP	691	44.487	1.165	16.367	1.00	20.88
ATOM	5400	CD1	TRP	691	42.791	-0.090	19.314	1.00	23.72
MOTA	5401	NEl	TRP	691	41.786	0.031	18.389	1.00	26.15
MOTA	5403	CZ2	TRP	691	41.704	0.788	15.997	1.00	25.07
MOTA	5404	CZ3	TRP	691	43.883	1.448	15.163	1.00	22.80
ATOM	5405	CH2	TRP	691	42.501	1.251	14.982	1.00	24.95
MOTA	5406	С	TRP	691	46.566	-1.116	17.811	1.00	30.63
ATOM	5407	0	TRP	691	45.943	-1.892	17.093	1.00	33.02
ATOM	5408	N	GLU	692	47.625	-0.431	17.386	1.00	31.00
MOTA	5410	CA	GLU	692	48.130	-0.545	16.018	1.00	29.00
MOTA	5411	CB	GLU	692	49.285	0.426	15.778	1.00	26.55

ATOM	5412	CG	GLU	692	48.873	1.876	15.651	1.00	29.90
MOTA	5413	CD	GLU	692	50.040	2.781	15.316	1.00	29.83
ATOM	5414	OE1	GLU	692	50.770	3.174	16.247	1.00	32.18
MOTA	5415	OE2	GLU	692	50.227	3.110	14.124	1.00	31.57
ATOM	5416	С	GLU	692	48.622	-1.959	15.735	1.00	29.02
ATOM	5417	0	GLU	692	48.474	-2.467	14.627	1.00	29.22
MOTA	5418	N	ILE	693	49.258	-2.573	16.724	1.00	29.54
ATOM	5420	CA	ILE	693	49.766	-3.933	16.555	1.00	31.01
MOTA	5421	СВ	ILE	693	50.634	-4.360	17.757	1.00	32.36
ATOM	5422	CG2	ILE	693	51.006	-5.845	17.641	1.00	34.39
ATOM	5423	CG1	ILE	693	51.909	-3.506	17.815	1.00	30.30
ATOM	5424	CD1	ILE	693	52.696	-3.693	19.082	1.00	25.66
ATOM	5425	С	ILE	693	`48.638	-4.939	16.381	1.00	30.63
MOTA	5426	0	ILE	693	48.633	-5.738	15.451		31.10
ATOM	5427	N	PHE	694	47.644	-4.858	17.248	1.00	32.60
ATOM	5429	CA	PHE	694	46.543	-5.793	17.172	1.00	33.86
ATOM	5430	СВ	PHE	694	45.938	-5.970	18.563	1.00	35.66
ATOM	5431	CG	PHE	694	46.941	-6.499	19.559	1.00	35.70
ATOM	5432	CD1	PHE	694	47.460	-5.684	20.556	1.00	37.18
ATOM	5433	CD2	PHE	694	47.449	-7.794	19.426	1.00	34.37
ATOM	5434	CE1	PHE	694	48.473	-6.150	21.392	1.00	36.90
MOTA	5435	CE2	PHE	694	48.456	-8.265	20.255	1.00	31.89
MOTA	5436	CZ	PHE	694	48.970	-7.446	21.234	1.00	34.95
ATOM	5437	C	PHE	694	45.532	-5.576	16.049	1.00	34.26
MOTA	5438	o	PHE	694	44.702	-6.442	15.787	1.00	37.52
MOTA	5439	N	THR	695	45.636	-4.441	15.359	1.00	32.23
ATOM	5441	CA	THR	695	44.775	-4.160	14.215	1.00	28.08
MOTA	5442	СВ	THR	695		-2.728	14.241	1.00	25.71
ATOM	5443	OG1	THR	695	45.237	-1.762	14.228	1.00	24.94
ATOM	5445	CG2	THR	695	43.353	-2.528	15.468	1.00	23.07
ATOM	5446	С	THR	695	45.615	-4.348	12.955	1.00	27.53
ATOM	5447	0	THR	695	45.166	-4.066	11.845	1.00	30.89
ATOM	5448	N	LEU	696	46.833	-4.848	13.145	1.00	27.73
ATOM	5450	CA	LEU	696	47.781	-5.081	12.061	1.00	28.99
ATOM	5451	СВ	LEU	696	47.370	-6.297	11.226	1.00	27.78
ATOM	5452	CG	LEU	696	47.379	-7.591	12.047	1.00	29.89
ATOM	5453	CD1	LEU	696	47.251	-8.823	11.164	1.00	29.96
ATOM	5454	CD2	LEU	696	48.668	~7.656	12.803	1.00	30.20
ATOM	5455	С	LEU	696	48.044	-3.853	11.179	1.00	30.33
ATOM	5456	0	LEU	696	48.006	-3.926	9.948	1.00	29.41
ATOM	5457	N	GLY	697	48.374	-2.738	11.831	1.00	30.92
MOTA	5459	CA	GLY	697	48.655	-1.503	11.113	1.00	30.35
ATOM	5460	С	GLY	697	47.420	-0.650	10.912	1.00	30.65
ATOM	5461	0	GLY	697	47.359	0.178	10.000	1.00	30.01
ATOM	5462	N	GLY	698	46.428	-0.836	11.772	1.00	30.50
MOTA	5464	CA	GLY	698	45.209	-0.063	11.656	1.00	30.36
ATOM	5465	C	GLY	698	45.416	1.415	11.930	1.00	30.07
ATOM	5466	0	GLY	698	46.320	1.809	12.666	1.00	30.56
ATOM	5467	N	SER	699	44.554	2.228	11.338	1.00	29.65
ATOM	5469	CA	SER	699	44.597	3.674	11.485	1.00	28.42
MOTA	5470	СВ	SER	699	44.263	4.324	10.145	1.00	24.61
MOTA	5471	OG	SER	699	43.960	5.693	10.280	1.00	31.25
ATOM	5473	c	SER	699	43.621	4.137	12.574	1.00	28.27
ATOM	5474	0	SER	699	42.406	3.930	12.474	1.00	
	/-	•	CLIK	000	74,700	3.330	14.4/7	1.00	27.14

MOTA	5475	N	PRO	700	44.160	4.682	13.675	1.00	29.29
ATOM	5476	CD	PRO	700	45.587	4.867	13.999	1.00	26.09
ATOM	5477	CA	PRO	700	43.303	5.155	14.764	1.00	29.30
ATOM	5478	CB	PRO	700	44.319	5.624	15.812	1.00	27.68
ATOM	5479	CG	PRO	700	45.531	5.982	14.985	1.00	27.85
ATOM	5480	С	PRO	700	42.413	6.305	14.306	1.00	29.71
ATOM	5481	0	PRO	700	42.800	7.096	13.446	1.00	31.38
ATOM	5482	N	TYR	701	41.204	6.357	14.854	1.00	29.51
ATOM	5484	CA	TYR	701	40.246	7.419	14.548	1.00	30.25
MOTA	5485	CB	TYR	701	40.559	8.647	15.405	1.00	33.50
MOTA	5486	CG	TYR	701	40.321	8.413	16.866	1.00	37.84
ATOM	5487	CD1	TYR	701	41.323	8.638	17.803	1.00	40.05
ATOM	5488	CE1	TYR	701	41.092	8.412	19.158	1.00	42.28
MOTA	_5489_	CD2	TYR	701	39.084	7.965	17.310	1.00	41.54.
MOTA	5490	CE2	TYR	701	38.845	7.738	18.653	1.00	43.70
ATOM	5491	CZ	TYR	701	39.845	7.963	19.574	1.00	42.63
MOTA	5492	OH	TYR	701	39.584	7.716	20.907	1.00	45.31
MOTA	5494	С	TYR	701	40.173	7.829	13.088	1.00	28.45
MOTA	5495	0	TYR	701	40.356.	9.001	12.760	1.00	29.03
MOTA	5496	N	PRO	702	39.901	6.867	12.191	1.00	28.05
ATOM	5497	CD	PRO	702	39.671	5.430	12.417	1.00	2690
АТОМ	5498	CA	PRO	702	39.815	7.181	10.764	1.00	27.48
ATOM	5499	CB	PRO	702	39.610	5.807	10.119	1.00	27.06
ATOM	5500	CG	PRO	702	38.923	5.036	11.169	1.00	28.28
ATOM	5501	C	PRO	702	38.689	8.145	10.440	1.00	26.81
ATOM	5502	0	PRO	702	37.554	7.953	10.865	1.00	26.26
ATOM	5503	N	GLY	703	39.035	9.192	9.693	1.00	28.48
MOTA	5505	CA	GLY	703	38.085	10.217	9.295	1.00	26.54
MOTA	5506	C	GLY	703	37.862	11.285	10.351	1.00	28.03
ATOM ATOM	5507	0	GLY	703	37.110	12.231	10.108	1.00	28.93
ATOM	5508 5510	N CA	VAL VAL	704 704	38.518	11.149	11.505	1.00	28.16
ATOM	5511	CB	VAL	704	38.369	12.081	12.619	1.00	29.55
ATOM	5512	CG1	VAL	704	38.473	11.360	13.984	1.00	28.50
ATOM	5513	CG2	VAL	704	38.330	12.350	15.135	1.00	28.07
ATOM	5514	C	VAL	704	37.403 39.375	10.295	14.091	1.00	29.78
ATOM	5515	o	VAL	704	40.578	13.227	12.588	1.00	32.00
ATOM	5516	N	PRO	705	38.888	13.028 14.446	12.758 12.336	1.00	33.85
MOTA	5517	CD	PRO	705	37.512	14.763	11.906	1.00 1.00	33.56
ATOM	5518	CA	PRO	705	39.745	15.628	12.280	1.00	33.69 32.65
ATOM	5519	CB	PRO	705	38.863	16.647	11.569	1.00	34.10
ATOM	5520	CG	PRO	705	37.478	16.256	12.021	1.00	36.38
MOTA	5521	c	PRO	705	40.164	16.081	13.668	1.00	33.22
ATOM	5522	0	PRO	705	39.549	15.708	14.668	1.00	33.26
ATOM	5523	N	VAL	706	41.198	16.912	13.710	1.00	34.61
ATOM	5525	CA	VAL	706	41.764	17.417	14.954	1.00	37.72
ATOM	5526	CB	VAL	706	42.803	18.527	14.673	1.00	39.14
MOTA	5527	CG1	VAL	706	43.483	18.941	15.957	1.00	39.12
ATOM	5528	CG2	VAL	706	43.836	18.038	13.670	1.00	41.07
ATOM	5529	c	VAL	706	40.740	17.934	15.969	1.00	38.70
MOTA	5530	0	VAL	706	40.761	17.536	17.136	1.00	38.42
ATOM	5531	N	GLU	707	39.834	18.796	15.517	1.00	40.43
ATOM	5533	CA	GLU	707	38.823	19.375	16.395	1.00	40.66
MOTA	5534	СВ	GLU	707	37.973	20.379	15.621	1.00	43.40
									

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MOTA 5535 GLU 707 С 37:940 18.316 17.028 1.00 41.03 MOTA 5536 0 GLU 707 37.642 18.370 18.231 1.00 41.52 MOTA 5537 N GLU 708 37.560 17.327 16.224 1.00 41.62 MOTA 16.243 5539 CA GLU. 708 36.708 16.700 1.00 41.06 5540 **MOTA** GLU 708 CB 36.179 15.425 15.523 1.00 45.19 ATOM 5541 CG GLU 708 35.281 14.571 16.221 1.00 48.74 MOTA GLU 5542 CD 708 34.063 16.825 15.258 1.00 57.18 **ATOM** 5543 OE1 GLU 708 33.523 16.203 16.207 1.00 54.30 MOTA 5544 GLU OE2 708 33.646 17.934 14.837 1.00 61.76 **ATOM** 5545 С GLU 708 37.443 15.363 17.694 1.00 38.39 **ATOM** 5546 GLU 708 0 36.867 14.927 18.696 1.00 36.76 **ATOM** 5547 LEU 709 N 38.725 15.131 17.434 1.00 37.78 ATOM 5549 CA LEU 709 39.555 14.327 18.324 1.00 38.13 **ATOM** 5550 CB LEU 709 41.007 14.255 17.920 1.00 35.45 **ATOM** 5551 LEU CG 709 41.984 13.560 18.786 1.00 35.57 **ATOM** 5552 CD1 LEU 709 41.825 12.049 18.729 1.00 32.33 **ATOM** 5553 CD2 LEU 709 43.407 13.965 18.484 1.00 31.98 MOTA 5554 LEU 39.550 С 709 14.945 19.716 1.00 38.31 MOTA 5555 LEU 0 709 39.362 14.250 20.717 1.00 38.16 MOTA 5556 N PHE 710 39.776 16.254 19.770 1.00 40.09 MOTA 5558 CA PHE 710 39.807 16.973 21.036 1.00 43.61 MOTA 5559 CB PHE 39.997 710 18.475 20.797 1.00 48.22 MOTA 5560 CG PHE 710 41.328 18.834 20.192 1.00 51.77 **ATOM** 5561 CD1 PHE 710 42.395 17.939 20.231 1.00 52.94 MOTA 5562 CD2 PHE 710 41.513 20.072 19.579 1.00 53.99 MOTA 5563 CE1 PHE 710 43.632 18.275 19.679 1.00 56.48 MOTA 5564 CE2 PHE 710 42.746 20.422 19.021 1.00 55.72 MOTA 5565 CZPHE 710 43.807 19.517 19.069 1.00 57.84 MOTA 5566 С PHE 710 38.519 16.726 21.796 1.00 43.35 **ATOM** 5567 O PHE 710 38.539 16.424 22.989 1.00 43.22 MOTA 5568 N LYS 711 37.399 16.8C4 21.083 1.00 44.68 MOTA 5570 CA LYS 711 36.095 16.587 21.690 1.00 43.47 ATOM 5571 CB LYS 711 34.977 16.878 20.687 1.00 44.33 16.765 **MOTA** 5572 CG LYS 711 33.601 21.299 1.00 47.63 **ATOM** 5573 CD LYS 711 32.510 17.206 20.362 1.00 49.97 **MOTA** 5574 CE LYS 711 31.158 16.873 29.960 1.00 51.70 ATOM 5575 NZ LYS 711 30.038 17.412 20.150 1.00 57.55 **ATOM** 5579 С LYS 711 35.986 15.173 22.261 1.00 42.72 ATOM 5580 0 LYS 711 35.589 14.999 23.420 1.00 41.16 MOTA 5581 N LEU 712 36.392 14.176 21.471 1.00 42.52 **ATOM** 5583 CA LEU 712 36.361 12.770 21.898 1.00 42.52 **ATOM** 5584 CB LEU 712 36.922 11.843 20.809 1.00 41.56 **ATOM** 5585 CG LEU 712 36.090 11.528 19.560 1.00 41.87 **ATOM** 5586 CD1 LEU 712 36.902 10.620 18.636 1.00 36.28 **ATOM** 5587 CD2 LEU 712 34.760 10.868 19.951 1.00 37.19 **ATOM** 5588 C LEU 712 37.158 12.564 23.180 1.00 42.34 **ATOM** 5589 0 LEU 712 36.697 11.886 24.107 1.00 40.77 ATOM 5590 N LEU 713 38.366 13.121 23.208 1.00 42.68 **ATOM** 5592 CA LEU 713 39.240 13.025 24.371 1.00 44.05 **ATOM** 5593 CB LEU 713 40.581 13.710 24.100 1.00 45.45 MOTA 5594 CG LEU 713 41.418 13.114 22.963 1.00 44.78 MOTA 5595 CD1 LEU 713 42.676 13.945 22.750 1.00 41.89 **ATOM** 5596 CD2 LEU 713 41.757 11.660 23.282 1.00 43.21 **ATOM** 5597 C LEU 713 38.571 13.654 25.591 1.00 44.66

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ATOM 5598 0 LEU 713 38.562 13.051 26.662 1.00 45.70 MOTA 5599 N LYS 714 37.980 14.839 25.418 1.00 43.05 MOTA 5601 CA LYS 714 37.300 15.510 26.524 1.00 42.19 MOTA 5602 CB LYS 714 36.884 16.921 26.127 1.00 42.41 **ATOM** 5603 LYS . CG 714 38.076 17.828 25.918 1.00 46.10 MOTA 5604 LYS CD 714 37.684 19.259 25.589 1.00 49.86 MOTA 5605 CE LYS 714 38.939 20.097 25.292 1.00 52.55 MOTA 5606 NZ LYS 714 39.889 20.148 26.459 1.00 50.17 **ATOM** 5610 C LYS 714 36.104 14.728 27.054 1.00 42.39 **ATOM** 5611 O LYS 714 35.767 1.00 14.824 28.237 43.44 MOTA 5612 N GLU 715 13.934 35.480 26.192 1.00 40.44 **ATOM** 5614 CA **GLU** 715 34.342 13.118 26.593 1.00 37.90 ATOM 5615 CB GLU 715 33.408 12.893 25.411 1.00 39.54 MOTA 5616 CG **GLU** 715 32.800 14.174 24.846 1.00 45.20 MOTA 5617 32.032 CD GLU 715 13.936 23.563 1.00 47.85 MOTA 5618 OE1 GLU 715 32.409 13.008 22.810 1.00 50.00 **ATOM** 5619 OE₂ GLU 715 31.061 14.677 23.304 1.00 50.41 ATOM 5620 C GLU 715 34.793 11.773 27.157 1.00 37.31 **ATOM** 5621 0 GLU 715 33.970 10.907 27.450 1.50 36.79 ATOM 5622 N GLY 716 36.102 11.585 27.286 1.00 36.60 MOTA 5624 CA GLY 716 36.623 10.336 27.819 1.00 37.11 MOTA 5625 C GLY 716 36.503 9.140 26.887 1.00 38.30 ATOM 5626 0 GLY 716 36.603 7.994 27.34C 1.00 36.84 **ATOM** 5627 N HIS 717 36.307 9.404 25.592 1.00 40.24 ATOM 5629 CA HIS 717 36.167 24.579 8.353 1.00 42.63 **ATOM** 5630 CB HIS 717 35.800 8.951 23.217 1.00 43.11 ATOM 5631 CG HIS 717 35.745 7.941 22.112 1.00 44.69 MOTA 5632 CD2 HIS 717 34.756 7.101 21.717 1.00 45.13 MOTA 5633 ND1 HIS 717 36.818 7.683 21.283 1.00 47.31 **ATOM** 5635 CE1 HIS 717 36.494 6.728 20.425 1.00 47.61 MOTA 5636 NE2 HIS 717 35.250 6.35? 20.670 1.00 44.95 MOTA 5638 C HIS 717 37.451 7.567 24.413 1.00 44.84 MOTA 5639 0 HIS 717 38.528 8.152 24.295 1.00 46.79 MOTA 5640 N ARG 718 37.313 6.247 24.337 1.00 45.44 **ATOM** 5642 CA ARG 718 38.440 5.345 24.170 1.00 45.36 ATOM 5643 CB ARG 718 38.614 4.496 25.434 1.00 43.82 MOTA 5644 CG ARG 718 38.976 5.308 26.697 1.00 44.52 MOTA 5645 CDARG 718 40.284 6.065 26.476 1.00 45.02 MOTA 5646 NE ARG 718 40.718 6.856 27.630 1.00 43.12 MOTA 5648 27.744 CZARG 718 40.550 8.173 1.00 44.77 **ATOM** 5649 NH1 ARG 718 39.940 8.859 26.784 1.00 44.67 MOTA 5652 NH2 ARG 718 41.067 8.826 28.777 1.00 46.39 MOTA 5655 C ARG 718 38.124 4.474 22.952 1.00 45.94 MOTA 5656 O ARG 718 36.953 4.243 22.645 1.00 47.59 MOTA 5657 N MET 719 39.145 4.077 22.204 1.00 45.34 MOTA 5659 CA MET 719 38.925 3.253 21.029 1.00 44.28 MOTA 5660 CB MET 719 40.198 3.125 20.185 1.00 42.30 MOTA 5661 CG MET 719 40.575 4.399 19.441 1.00 38.44 MOTA 5662 SD 719 MET 42.000 4.225 18.368 1.00 36.97 5663 MOTA CE MET 719 43.317 4.219 19.511 1.00 36.09 MOTA 5664 C MET 719 38.415 1.877 21.418 1.00 46.21 MOTA 5665 0 MET 719 38.708 1.393 22.517 1.00 43.29 MOTA 5666 N ASP 720 37.659 1.267 20.498 1.00 48.79 MOTA 5668 CA ASP 720 37.069 -0.063 20.666 1.00 48.87

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ATOM	5669	CB	ASP	720	36.099	-0.369	19.513	1.00	54.01
ATOM	5670	CG	ASP	720	34.766	0.374	19.632	1.00	59.30
ATOM	5671	OD1	ASP	720	34.762	1.583	19.981	1.00	62.96
ATOM	5672	OD2	ASP	720	33.716	-0.259	19.354	1.00	58.64
MOTA	5673	C	ASP	720	38.126	-1.154	20.688	1.00	46.10
ATOM	5674	0	ASP	720	39.213	-0.992	20.125	1.00	44.13
ATOM	5675	N	LYS	721	37.788	-2.272	21.322	1.00	45.27
ATOM	5677	CA	LYS	721	38.689	-3.413	21.404	1.00	43.25
ATOM	5678	СВ	LYS	721	38.172	-4.436	22.416	1.00	42.02
ATOM	5679	CG	LYS	721	39.072	-5.651	22.557	1.00	46.57
MOTA	5680	CD	LYS	721	38.602	-6.576	23.666	1.00	49.96
ATOM	5681	CE	LYS	721	38.300	-7.971	23.141	1.00	51.80
ATOM	5682	NZ	LYS	721	37.937	8.920	24.240	1.00	56.08
ATOM	5686	C	LYS	721	38.769	-4.055	20.031	1.00	43.67
ATOM	5687	0	LYS	721	37.736	-4.313	19.394	1.00	44.02
ATOM	5688	N	PRO	722	39.995	-4.233	19.513	1.00	43.94
MOTA	5689	CD	PRO	722	41.281	-3.711	20.001	1.00	45.90
ATOM	5690	CA	PRO	722	40.159	-4.853	18.198	1.00	43.96
ATOM	5691	СВ	PRO	722	41.665	-4.720	17.941	1.00	43.11
ATOM	5692	CG	PRO	722	42.046	-3.509	18.715	1.00	45.16
ATOM	5693	С	PRO	722	39.772	-6.317	18.295	1.00	43.09
ATOM	5694	o	PRO	722	39.764	-6.888	19.385	1.00	41.32
MOTA	5695	N	SER	723	39.382		17.170	1.00	45.79
ATOM	5697	CA	SER	723	39.044	-9.316	17.144	1.00	46.67
ATOM	5698	СВ	SER	723	38.303	-8.664	15.357	1.00	44.69
ATOM	5699	OG	SER	723	39.131	-8.414	14.736	1.00	49.79
ATOM	5701	С	SER	723	40.422	-8.961	17.146	1.00	46.90
ATOM	5702	O	SER	723	41.360	-9.411	16.581	1.00	48.81
MOTA	5703	N	ASN	724	40.540	-30.131	17.760	1 00	49.28
ATOM	5705	CA	ASN	724	41.826	-10.804	17.849	1.00	52.10
ATOM	5706	СВ	ASN	724	42.480	-10.947	16.469	1.00	55.86
ATOM	5707	CG	ASN	724	41.774	-11.957	15.592	1.60	58. 7 2
ATOM	5708	OD1	ASN	724	41.686	-13.140	15.941	1.00	62.28
ATOM	5709	ND2	ASN	724	41.258	-11.503	14.449	1.00	59.56
MOTA	5712	С	ASN	724	42.665	-9.931	18.770	1.00	51.97
ATOM	5713	0	ASN	724	43.621	-9.274	18.369	1.00	53.85
MOTA	5714	N	CYS	725	42.202	-9.859	20.004	1.00	51.02
ATOM	5716	CA	CYS	725	42.853	-9.094	21.049	1.00	50.18
MOTA	5717	CB	CYS	725	42.708	-7.583	20.811	1.00	47.75
ATOM	5718	SG	CYS	725	43.424	-6.577	22.130	1.00	44.37
MOTA	5719	С	CYS	725	42.131	-9.507	22.315	1.00	49.31
MOTA	5720	0	CYS	725	40.916	-9.371	22.417	1.00	49.90
MOTA	5721	N	THR	726	42.866	-10.088	23.249	1.00	48.52
MOTA	5723	CA	THR	726	42.262	-10.541	24.490	1.00	49.58
ATOM	5724	CB	THR	726	43.251	-11.444	25.291	1.00	49.84
MOTA	5725	OG1	THR	726	44.236	-10.648	25.976	1.00	49.05
MOTA	5727	CG2	THR	726	43.982	-12.363	24.352	1.00	47.96
ATOM	5728	С	THR	726	41.788	-9.369	25.356	1.00	49.93
MOTA	5729	0	THR	726	42.305	-8.256	25.244	1.00	51.55
ATOM	5730	N	ASN	727	40.829	-9.622	26.242	1.00	50.48
ATOM	5732	CA	ASN	727	40.335	-8.577	27.144	1.00	52.17
ATOM	5733	СВ	ASN	727	39.190	-9.099	28.016	1.00	57.57
ATOM	5734	CG	ASN	727	39.533	-10.409	28.714	1.00	66.49
ATOM	5735	OD1	ASN	727	40.709	-10.786	28.833	1.00	70.43
•		-					20.000	1.00	,0.33

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MOTA 5736 · ND2 ASN 727 38.500 -11.122 29.175 1.00 68.43 MOTA 5739 С ASN 727 41.491 -8.091 28.023 1.00 50.29 ATOM 5740 0 ASN 727 41.467 -6.976 28.540 1.00 49.88 **ATOM** 5741 N GLU 728 42.518 -8.927 28.163 1.00 50.60 **ATOM** 5743 CA GLU 728 43.700 -8.597 28.956 1.00 49.33 MOTA 5744 CB GLU 728 44.529 -9.859 29.220 1.00 50.44 MOTA 5745 CG GLU 728 45.802 -9.600 30.008 1.00 55.30 MOTA 5746 CD GLU 728 46.577 -10.862 30.354 1.00 57.40 MOTA 5747 OE1 GLU 728 46.716 -11.754 29.489 1.00 56.75 MOTA 5748 OE2 GLU 728 47.062 -10.950 31.502 1.00 59.85 MOTA 5749 C GLU 728 44.539 -7.552 28.212 1.00 47.08 MOTA 5750 0 GLU 728 44.888 48.02 -6.512 28.776 1.00 MOTA 5751 N LEU 729 44.846 -7.821 1.00 26.945 43.34 MOTA 5753 LEU CA 729 45.630 -6.891 26.129 1.00 42.01 MOTA 5754 CB LEU 729 45.899 -7.500 24.751 1.00 39.46 ATOM 5755 CG LEU 729 46.911 -8.639 24.772 1.00 40.31 MOTA 5756 CD1 LEU 729 46.782 -9.482 23.531 1.00 42.21 MOTA 5757 CD2 LEU 729 48.314 -8.068 24.900 1.00 42.49 **MOTA** 5758 С LEU 729 44.901 -5.557 25.980 1.00 40.61 **ATOM** 5759 0 LEU 729 45.510 -4.481 25.953 1.00 38.33 **ATOM** 5760 N TYR 730 43.580 -5.637 25.909 1.00 39.07 MOTA 5762 CA TYR 730 42.761 -4.455 25.773 1.00 38.61 ATOM 5763 CB TYR 730 41.341 -4.837 25.369 1.00 36.79 MOTA 5764 CG TYR 730 40.454 -3.646 25.125 1.00 37.08 MOTA 5765 CD1 TYR 730 40.760 -2.721 24.127 1.00 32.86 ATOM 5766 CEl TYR 730 39.961 -1.616 23.912 1.00 29.79 MOTA 5767 CD2 TYR 730 39.328 -3.420 25.916 1.00 36.99 MOTA 5768 CE2 730 TYR 38.522 -2.312 25.704 1.00 36.69 MOTA 5769 CZTYR 730 38.853 -1.412 24.706 1.00 32.69 MOTA 5770 OH TYR 730 38.044 -0.320 24.492 1.00 38.80 MOTA 5772 С TYR 730 42.767 -3.662 27.080 1.00 39.75 MOTA 5773 0 TYR 730 42.781 -2.430 27.065 1.00 40.53 MOTA 5774 N MET 731 42.738 -4.360 28.210 1.00 41.88 MOTA 5776 CA MET 731 42.778 -3.684 29.509 1.00 45.34 **ATOM** 5777 CB MET 731 42.658 -4.697 30.646 1.00 53.46 MOTA 5778 CG -5.248 MET 731 41.253 30.836 1.00 64.30 MOTA 5779 SD MET 731 40.134 -4.095 31.653 1.00 75.78 MOTA 5780 CE MET 731 40.657 -4.338 1.00 69.70 33.370 MET MOTA 5781 С 731 44.099 -2.927 1.00 29.614 41.53 **ATOM** 5782 0 MET 731 44.157 -1.814 30.138 1.00 37.91 **ATOM** 5783 N MET 732 45.156 -3.545 29.098 1.00 40.48 **ATOM** 5785 CA MET 732 46.478 -2.937 29.091 1.00 40.23 **MOTA** 5786 CB MET 732 47.508 -3.872 28.436 1.00 40.29 MOTA 5787 CG MET 732 48.929 -3.307 28.390 1.00 38.07 MOTA 5788 SD MET 732 50.171 -4.522 27.908 1.00 37.65 MOTA 5789 CE MET 732 50.407 -5.343 29.431 1.00 37.90 **ATOM** 5790 С MET 732 46.378 -1.623 28.317 1.00 38.96 MOTA 5791 0 MET 732 46.843 -0.591 28.790 1.00 41.36 MOTA 5792 MET N 733 45.744 -1.663 27.148 1.00 36.94 MOTA 5794 CA MET 733 45.574 -0.463 26.340 1.00 35.19 MOTA 5795 44.796 CB MET -0.769 733 25.070 1.00 36.07 MOTA 5796 CG MET 45.549 733 -1.577 24.048 1.00 35.99 MOTA 5797 SD MET 733 44.471 -1.851 22.641 1.00 40.05 MOTA 5798 CE MET 733 45.244 -3.351 21.909 1.00 33.13

MOTA	5799	С	MET	733	44.800	0.560	27.141	1.00	37.29
MOTA	5800	0	MET	733	45.207	1.719	27.245	1.00	39.14
ATOM	5801	N	ARG	734	43.690	0.125	27.735	1.00	38.76
MOTA	5803	CA	ARG	734	42.849	1.014	28.532	1.00	39.49
MOTA	5804	CB	ARG	.734	41.577	0.297	28.993	1.00	40.33
MOTA	5805	CG	ARG	734	40.699	-0.225	27.856	1.00	38.02
MOTA	5806	CD	ARG	734	40.256	0.877	26.909	1.00	42.72
MOTA	5807	NE	ARG	734	39.443	1.898	27.567	1.00	48.85
MOTA	5809	CZ	ARG	734	38.120	1.838	27.700	1.00	52.35
ATOM	5810	NH1	ARG	734	37.435	0.811	27.222	1.00	54.79
ATOM	5813	NH2	ARG	734	37.477	2.804	28.338	1.00	54.69
MOTA	5816	C	ARG	734	43.627	1.587	29.715	1.00	38.70
ATOM	5817	0	ARG	734	43.445	2.757	30.068	1.00	40.92
ATOM	5818	N	ASP	735	44.530	0.782	30:276	1.00	38.76
ATOM	5820	CA	ASP	735	45.379	1.208	31.399	1.90	38.60
MOTA	5821	CB	ASP	735	46.325	0.087	31.825	1.00	41.34
MOTA	5822	CG	ASP	735	45.622	-1.022	32.574	1.00	44.66
ATOM	5823	OD1	ASP	735	46.048	-2.194	32.428	1.00	43.15
MOTA	5824	OD2	ASP	735	44.657	-0.713	33.313	1.00	44.46
MOTA	5825	С	ASP	735	46.215	2.385	30.938	1.00	37.76
ATOM	5826	0	ASP	735	46.235	3.446	31.585	1.00	36.35
ATOM	5827	N	CYS	736	46.890	2.182	29.805	1.00	35.39
ATOM	5829	CA	CYS	736	47.730	3.196	29.181	1.00	34.77
MOTA	5830	CB	CYS	736	48.379	2.652.	27.916	1.00	30.62
MOTA	5831	SG	CYS	736	49.453	1.261	28.198	1.00	30.96
MOTA	5832	C	CYS	736	46.938	4.429	28.814	1.00	35.98
ATOM	5833	0	CYS	736	47.516	5.491	28.606	1.00	37.38
MOTA	5834	N	TRP	737	45.620	4.290	28.713	1.00	38.50
MOTA	5836	CA	TRP	737	44.772	5.423	28.370	1.00	40.16
MOTA	5837	CB	TRP	737	43.791	5.028	27.271	1.00	38.41
MOTA	5838	CG	TRP	737	44.453	4.586	26.011	1.00	39.33
ATOM	5839	CD2	TRP	737	43.893	3.718	25.020	1.00	39.64
ATOM	5840	CE2	TRP	737	44.852	3.583	23.992	1.00	39.97
MOTA	5841	CE3	TRP	737	42.672	3.040	24.900	1.00	37.06
MOTA	5842	CD1	TRP	737	45.695	4.932	25.556	1.00	39.56
MOTA	5843	NE1	TRP	737	45.941	4.336	24.343	1.00	38.61
MOTA	5845	CZ2	TRP	737	44.627	2.795	22.859	1.00	38.78
ATOM	5846	CZ3	TRP	737	42.452	2.261	23.778	1.00	38.90
ATOM	5847	CH2	TRP	737	43.426	2.145	22.772	1.00	38.18
MOTA	5848	C	TRP	737	44.028	6.029	29.563	1.00	41.30
ATOM	5849	O	TRP	737	42.979	6.658	29.398	1.00	41.45
ATOM	5850	И	HIS	738	44.575	5.873	30.763	1.00	43.01
MOTA	5852	CA	HIS	738	43.932	6.423	31.948	1.00	44.64
ATOM	5853	CB	HIS	738	44.454	5.735	33.205	1.00	46.20
MOTA	5854	CG	HIS	738	43.742	6.154	34.458	1.00	50.35
MOTA	5855	CD2	HIS	738	43.473	7.379	34.963	1.00	49.09
ATOM	5856	ND1	HIS	738	43.220	5.244	35.355	1.00	49.94
ATOM	5858	CE1	HIS	738	42.659	5.899	36.357	1.00	52.92
MOTA	5859	NE2	HIS	738	42.798	7.194	36.146	1.00	46.91
MOTA	5861	С	HIS	738	44.174	7.921	32.037	1.00	45.26
MOTA	5862	0	HIS	738	45.314	8.356	32.021	1.00	45.31
ATOM	5863	N	ALA	739	43.099	8.686	32.224	1.00	46.61
MOTA	5865	CA	ALA	739	43.155	10.150	32.322	1.00	48.49
MOTA	5866	СВ	ALA	739	41.823	10.681	32.790	1.00	49.69

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ATOM	5867	C	ALA	739	44.272	10.682	33.224	1.00	50.77
MOTA	5868	0	ALA	739	45.004	11.601	32.846	1.00	51.77
MOTA	5869	N	VAL	740	44.336	10.138	34.439	1.00	51.47
MOTA	5871	CA	VAL	740	45.352	10.485	35.439	1.00	51.09
MOTA	5872	CB	VAL	740	44.897	10.075	36.850	1.00	52.40
MOTA	5873	CG1	VAL	740	45.847	10.624	37.878	1.00	53.38
MOTA	5874	CG2	VAL	740	43.485	10.544	37.105	1.00	55.18
ATOM	5875	С	VAL	740	46.649	9.727	35.130	1.00	48.99
ATOM	5876	0	VAL	740	46.773	8.534	35.440	1.00	47.72
ATOM	5877	N	PRO	741	47.646	10.421	34.565	1.00	48.31
MOTA	5878	CD	PRO	741	47.603	11.861	34.253	1.00	47.84
ATOM	5879	CA	PRO	741	48.949	9.852	34.197	1.00	48.51
MOTA	5880	CB	PRO	741	49.762	11.087	33.828	1.00	46.83
MOTA	5881	CG	PRO	741	48.714	12.000	33.255	1.00	.46.21
MOTA	5882	C	PRO	741	49.641	9.016	35.275	1.00	49.12
ATOM	5883	O	PRO	741	50.449	8.139	34.955	1.00	46.57
MOTA	5884	N	SER	742	49.327	9.290	36.541	1.00	49.47
ATOM	5886	CA	SER	742	49.928	8.557	37.651	1.00	49.50
MOTA	5887	CB	SER	742	49.760	9.326	38.963	1.00	51.06
MOTA	5888	OG	SER	742	48.403	9.638	39.209	1.00	53.81
ATOM	5890	C	SER	742	49.339	7.159	37.787	1.00	48.81
ATOM	5891	0	SER	742	49.926	6.284	38.427	1.00	49.45
MOTA	5892	N	GLN	743	48.164	6.959	37.203	1.00	47.82
MOTA	5894	CA	GLN	743	47.529	5.658	37.273	1.00	46.34
ATOM	5895	CB	GLN	743	46.022	5.791	37.432	1.00	49.74
ATOM	5896	CG	GLN	743	45.519	5.305	38.784	1.00	55.41
ATOM	5897	CD	GLN	743	46 178	5.030	39.947	1.00	59.15
MOTA	5898	OE1	GLN	743	46.905	5.425	40.748	1.00	59.02
ATOM	5899	NE2	GLN	743	45.922	7.338	40.052	1.00	60.03
ATOM	5902	C	GLN	743	47.874	4.768	36.095	1.00	44.34
ATOM	5903	0	GLN	743	47.548	3.578	36.114	1.00	44.64
ATOM ATOM	5904	N Ca	ARG	744	48.497	5.339	35.059	1.00	42.83
ATOM	5906 5907	CA CB	ARG	744	48.914	4.559	33.880	1.00	40.34
ATOM	5908	CG	ARG ARG	744 744	49.349	5.469	32.724	1.00	35.84
ATOM	5909	CD	ARG	744	48.296	6.406	32.190	1.00	28.25
ATOM	5910	NE	ARG	744	48.906 47.948	7.383	31.216	1.00	22.56
ATOM	5912	CZ	ARG	744		8.437	30.922	1.00	28.09
ATOM	5913	NH1	ARG	744	48.258 49.524	9.658	30.493	1.00	32.83
ATOM	5916	NH2	ARG	744	47.307	10.001 10.569	30.278 30.360	1.00	34.44
ATOM	5919	C	ARG	744	50.110	3.712	34.295	1.00	32.00
MOTA	5920	o	ARG	744	50.906	4.124	35.145	1.00	41.58
ATOM	5921	N	PRO	745	50.223	2.489	33.754	1.00	45.48 40.97
ATOM	5922	CD	PRO	745	49.345	1.749	32.831	1.00	
ATOM	5923	CA	PRO	745	51.381	1.685	34.157	1.00	39.90
ATOM	5924	СВ	PRO	745	51.063	0.311	33.558		39.77
ATOM	5925	CG	PRO	745	50.255	0.642		1.00	39.31
ATOM	5926	C	PRO	745	52.664	2.269	32.344	1.00	40.98
ATOM	5927	0	PRO	745	52.631	3.009	33.573 32.595	1.00	38.44
ATOM	5928	N	THR	746	53.783	2.001	34.224	1.00	39.64
ATOM	5930	CA	THR	746	55.066	2.462		1.00	37.50
ATOM	5931	CB	THR	746	56.108	2.462	33.728 34.869	1.00	37.56
ATOM	5932	OG1	THR	746	56.286	1.285	35.487	1.00	38.58
ATOM	5934	CG2	THR	746	55.666	3.567	35.487	1.00	43.28
	2237	CUZ	1111	140	33.000	3.30/	33.033	1.00	34.64

MOTA	5935	С	THR	746	55.546	1.393	32.739	1.00	36.49
ATOM	5936	0	THR	746	55.118	0.234	32.817	1.00	34.18
ATOM	5937	N	PHE	747	56.453	1.768	31.839	1.00	35.27
ATOM	5939	CA	PHE	747	56.995	0.814	30.880	1.00	33.48
MOTA	5940	CB	PHE	747	58.025	1.475.	29.970	1.00	34.35
ATOM	5941	CG	PHE	747	57.419	2.369	28.920	1.00	32.49
MOTA	5942	CD1	PHE	747	56.715	1.825	27.856	1.00	30.69
ATOM	5943	CD2	PHE	747	57.519	3.749	29.018	1.00	32.81
MOTA	5944	CE1	PHE	747	56.122	2.639	26.907	1.00	29.41
ATOM	5945	CE2	PHE	747	56.926	4.573	28.072	1.00	32.93
MOTA	5946	CZ	PHE	747	56.223	4.014	27.015	1.00	31.50
ATOM	5947	С	PHE	747	57.621	-0.363	31.606	1.00	34.65
MOTA	5948	0	PHE	747	57.616	-1.474	31.099	1.00	36.34
ATOM	5949	Ŋ	LYS	.7.48	58.142	-0.128	32.808	1.00	37.75
MOTA	5951	CA	LYS	748	58.748	-1.205	33.583	1.00	39.67
ATOM	5952	CB	LYS	748	59.382	-0.664	34.873	1.00	43.06
MOTA	5953	CG	LYS	748	59.958	-1.757	35.774	1.00	48.96
MOTA	5954	CD	LYS	748	60.750	-1.207	36.966	1.00	52.20
MOTA	5955	CE	LYS	748	61.183	-2.344	37.907	1.00	53.62
ATOM	5956	NZ	LYS	748	62.057	-1.893	39.031	1.00	54.82
MOTA	5960	C	LYS	748	57.680	-2.263	33.882	1.00	39.65
MOTA	5961	O.	LYS	748	57.902	-3.454	33.652	1.00	38.91
ATOM	5962	И	GLN	749	56.503	-1.818	34.331	1.00	39.39
MOTA	5964	CA	GLN	749	55.402	-2.742	34.623	1.00	40.70
MOTA	5965	CB	GLN	749	54.177	-1.991	35.140	1.00	43.82
ATOM	5966	CG	GLN	749	54.395	-1.149	36.373	1.00	50.97
MOTA	5967	CD	GLN	749	53.175	-0.304	36.715	1.00	55.53
ATOM	5968	OE1	GLN	749	53.272	0.914	36.895	1.00	55.80
MOTA	5969	NE2	GLN	749	52.012	-0.940	36.773	1.00	60.05
MOTA	5972	C	GLN	749	55.009	-3.455	33.334	1.00	40.03
MOTA	5973	O	GLN	749	54.903	-4.679	33.298	1.00	40.26
MOTA	5974	N	LEU	750	54.802	-2.666	32.278	1.00	39.18
ATOM	5976	CA	LEU	750	54.400	-3.171	30.964	1.00	36.65
ATOM	5977	CB	LEU	750	54.369	-2.039	29.927	1.00	34.58
MOTA	5978	CG	LEU	750	53.355	-0.910	30.116	1.00	32.52
ATOM	5979	CD1	LEU	750	53.644	0.210	29.125	1.00	31.67
MOTA	5980	CD2	LEU	750	51.947	-1.435	29.935	1.00	31.37
MOTA	5981	С	LEU	750	55.321	-4.255	30.477	1.00	35.81
MOTA	5982	0	LEU	750	54.856	-5.267	29.963	1.00	35.81
MOTA	5983	N	VAL	751	56.626	-4.035	30.620	1.00	37.38
ATOM	5985	CA	VAL	751	57.607	-5.029	30.193	1.00	38.66
MOTA	5986	CB	VAL	751	59.077	-4.545	30.411	1.00	35.42
MOTA	5987	CG1	VAL	751	60.075	-5.646	30.041	1.00	29.83
MOTA	5988	CG2	VAL	751	59.342	-3.324	29.559	1.00	29.95
MOTA	5989	С	VAL	751	57.337	-6.314	30.974	1.00	41.63
ATOM	5990	0	VAL	751	57.312	-7.401	30.396	1.00	42.43
ATOM	5991	N	GLU	752	57.051	-6.174	32.267	1.00	43.35
ATOM	5993	CA	GLU	752	56.766	-7.329	33.111	1.00	47.39
MOTA	5994	CB	GLU	752	56.674	-6.914	34.587	1.00	50.66
MOTA	5995	CG	GLU	752	57.950	-6.243	35.101	1.00	54.77
MOTA	5996	CD	GLU	752	58.006	-6.101	36.612	1.00	55.14
MOTA	5997	OE1	GLU	752	58.246	-4.972	37.102	1.00	54.14
MOTA	5998	OE2	GLU	752	57.844	-7.131	37.308	1.00	57. 7 3
MOTA	5999	C	GLU	752	55.496	-8.068	32.655	1.00	46.00

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ATOM 6000 GLU 752 55.548 -9.261 32.328 0 1.00 46.25 MOTA 6001 ASP N 753 54.380 -7.346 32.601 1.00 44.35 **ATOM** 6003 ASP CA 753 53.099 -7.912 32.180 1.00 44.19 **ATOM** 6004 CB ASP 753 52.059 -6.814 31.985 1.00 46.22 **ATOM** 6005 **ASP** -6.279 CG 753 51.512 33.278 1.00 50.48 **ATOM** 6006 OD1 ASP 753 51.396 -7.062 34.248 1.00 52.15 **ATOM** 6007 OD2 ASP 753 51.170 -5.069 52.20 33.306 1.00 MOTA 6008 ASP C 753 53.244 -B.608 30.849 1.00 44.54 **ATOM** 6009 ASP 0 753 52.770 -9.724 30.674 1.00 46.03 MOTA 6010 N LEU 754 53.880 -7.918 29.906 1.00 44.43 MOTA 6012 CA LEU 754 54.079 -8.438 28.563 1.00 43.70 MOTA 6013 CB LEU 54.570 754 -7.339 27.618 1.00 43.48 MOTA 6014 CG LEU 754 53.481 -6.350 27.201 + 1.00 44.67 **ATOM** 6015 CD1 LEU 754 54.095 -5.218 26.399 1.00 44.51 **ATOM** 6016 CD2 LEU 754 52.384 -7.069 26.408 1.00 42.07 **ATOM** 6017 С LEU 754 54.993 -9.642 28.512 1.00 43.14 **ATOM** 6018 0 LEU 754 27.697 54.795 -10.536 1.00 41.32 **ATOM** 6019 N ASP 755 55.990 -9.671 29.383 1.00 44.74 **ATOM** 6021 ASP 755 CA 56.897 -10.800 29.426 1.00 47.24 **ATOM** 6022 CB ASP 755 57.942 -10.575 30.517 1.00 51.26 **ATOM** 6023 CG ASP 755 59.121 -11.518 30.407 1.00 55.39 **ATOM** 6024 OD1 ASP 755 59.739 -11.793 31.455 1.00 60.61 **ATOM** 6025 OD2 ASP 755 59.443 ~11.970 29.283 1.00 57.16 **ATOM** 6026 C ASP 755 56.023 -12.005 29.771 1.00 47.67 **ATOM** 6027 О ASP 755 56.041 -13.032 29.081 1.00 45.99 6028 MOTA N ARG 756 55.186 -11.816 30.789 1.00 46.72 **ATOM** 6030 CA **ARG** 756 54.272 -12.851 31.256 1.30 46.25 **ATOM** 6031 CB ARG 53.519 756 -12.36832.499 1.00 46.31 **ATOM** 6032 CG ARG 756 52.391 -13.297 32.953 1.00 46.99 ATOM 6033 CD ARG 756 51.733 -12.776 34.227 1.00 48.10 MOTA 6034 NE ARG 756 51.320 -11.379 34.118 1.00 53.67 MOTA 6036 CZ ARG 50.294 756 -10.951 33.385 1.00 55.35 ATOM 6037 NHl ARG 756 49.562 -11.812 32.684 1.00 54.10 MOTA 6040 NH2 ARG 756 50.008 -9.654 33.344 1.00 56.02 ATOM 6043 C ARG 756 53.282 -13.261 30.175 1.00 45.05 ATOM 6044 0 ARG 756 53.213 -14.429 29.806 1.00 47.19 ATOM 6045 757 N ILE 52.550 -12.289 29.647 1.00 43.47 MOTA 6047 CA ILE 757 51.552 -12.553 28.617 1.00 43.80 **ATOM** 6048 CB ILE 757 50.842 -11.241 28.161 1.00 42.02 MOTA 6049 CG2 ILE 757 49.811 -11.536 27.086 1.00 39.63 **ATOM** 6050 CG1 ILE 757 50.154 -10.578 29.361 1.00 40.00 **ATOM** 6051 CD1 ILE 757 49.600 -9.212 29.086 1.00 42.68 ATOM 6052 C ILE 757 52.148 -13.296 27.428 1.00 46.03 **ATOM** 6053 O ILE 757 51.549 -14.250 26.947 1.00 47.78 MOTA 6054 N VAL 758 53.359 -12.925 27.015 1.00 49.03 **ATOM** 6056 CA VAL 758 54.015 -13.584 25.884 1.00 51.51 **ATOM** 6057 CB VAL 758 55.412 -12.971 25.556 1.00 50.75 MOTA 605B CG1 VAL 758 56.105 -13.780 24.470 1.00 50.31 **ATOM** 6059 CG2 VAL 758 55.269 -11.541 25.081 1.00 52.52 6060 MOTA VAL 758 C 54.209 -15.050 26.212 1.00 54.30 MOTA 6061 VAL 758 0 53.991 -15.915 25.369 1.00 54.80 ATOM 6062 N ALA 759 54.617 -15.311 27.450 1.00 57.65 MOTA 6064 CA 759 ALA 54.858 -16.667 27.919 1.00 60.62 MOTA 6065 СВ ALA 759 55.423 -16.637 29.327 1.00 60.32

ATOM	6066	С	ALA	759	53.571	-17.478	27.889	1.00	63.25	
ATOM	6067	0	ALA	759	53.568	-18.638	27.478	1.00	65.81	
ATOM	6068	N	LEU	760	52.475	-16.856	28.305	1.00	63.56	
ATOM	6070	CA	LEU	760	51.191	-17.533	28.333	1.00	64.25	
MOTA	6071	CB	LEU	760	50.302	-16.912	29.407	1.00	65.66	
ATOM	6072	CG	LEU	760	50.894	-16.962	30.820	1.00	65.62	
MOTA	6073	CD1	LEU	760	49.988	-16.246	31.809	1.00	64.75	
ATOM	6074	CD2	LEU	760	51.109	~18.410	31.227	1.00	66.65	
ATOM	6075	C	LEU	760	50.483	-17.535	26.984	1.00	64.89	
MOTA	6076	0	LEU	760	49.390	-18.088	26.860	1.00	66.37	
MOTA	6077	N	THR	761	51.103	-16.933	25.973	1.00	65.24	
ATOM	6079	CA	THR	761	50.516	-16.882	24.634	1.00	64.44	
MOTA	6080	CB	THR	761	50.829	-15.539	23.925	1.00	62.95	
MOTA	6081	OG1	THR	761	50.247	14.463	24.669	1.00	62.70	
ATOM	60B3	CG2	THR	761	50.249	-15.525	22.521	1.00	60.59	
MOTA	6084	C	THR	761	51.003	-18.044	23.769	1.00	64.71	
MOTA	6085	0	THR	761	52.202	-18.201	23.533	1.00	64.70	
MOTA	6086	SG	CYS	1603	18.536	-8.819	20.295	0.50	33.97	PRT2
MOTA	6087	CG	MET	534	69.178	12.159	22.968	0.50	31.30	
MOTA	6088	SD	MET	534	68.892	13.138	24.442	0.50	33.06	
MOTA	6089	CE	MET	534	70.060	12.456	25.568	0.50	34.22	
MOTA	6090	SG	CYS	603	56.041	-7.885	16.319	0.50	37.82	
MOTA	2682	OH2	TIP3	1	71.788	25.340	2.479	1.00	24.18	
MOTA	2685	OH2	TIP3	2	40.022	4.089	16.127	1.00	43.09	
ATOM	2688	OH2	TIP3	3	83.745	19.577	10.510	1.00	27.38	
MOTA	2691	OH2	TIF3	4	83.420	20.163	7.482	1.00	30.85	
ATOM	2694	OH2	TIP3	5	75.022	16.439	6.505	1.00	33.15	
MOTA	2697	OH2	TIP3	6	86,308	19.567	9.284	1.00	33.55	
MOTA	2700	OH2	TIP3	7	51.888	11.346	24.141	1.00	34.30	
MOTA	2703	OH2	TIP3	8	55.125	9.616	22.499	1.00	21.44	
MOTA	2706	OH2	TIP3	9	57.087	4.925	32.412	1.00	28.79	
MOTA	2709	OH2	TIP3	10	52.142	4.824	13.180	1.00	21.14	
MOTA	2712	OH2	TIP3	11	41.312	5.600	22.910	1.00	49.23	
MOTA	2715	OH2	TIP3	12	45.083	9.130	21.671	1.00	37.09	
MOTA	2718	OH2	TIP3	13	64.608	-2.335	28.803	1.00	44.31	
MOTA	2721	OH2	TIP3	14	77.192	13.199	23.753	1.00	32.96	
ATOM	2724	OH2	TIP3	15	79.201	17.296	17.997	1.00	38.51	
ATOM	2727	OH2	TIP3	16	82.988	11.608	15.745	1.00	27.56	
MOTA	2730	OH2	TIP3	17	14.096	-9.819	0.333	1.00	23.53	
ATOM	2733	OH2	TIP3	18	38.325	0.249	5.313	1.00	43.17	
ATOM ATOM	2736	OH2	TIP3		26.939	6.001	5.100	1.00	30.00	
ATOM	2739	OH2	TIP3		34.305	-1.615	16.952	1.00	44.82	
ATOM	2742	OH2	TIP3		20.300	2.328	27.798	1.00	45.23	
	2745	OH2	TIP3		50.996	-11.607	38.052	1.00	43.49	
ATOM ATOM	2748	OH2	TIP3		17.261	-6.167	-1.444	1.00	27.13	
MOTA	2751	OH2	TIP3		27.724	8.124	14.996	1.00	31.20	
ATOM	2754	OH2	TIP3		31.558	0.294	6.872	1.00	34.54	
ATOM	2757	OH2	TIP3		26.907	-12.815	28.161	1.00	49.20	
	2760	OH2	TIP3		28.705	-17.192	13.269	1.00	30.16	
ATOM	2763	OH2	TIP3		88.639	13.953	7.692	1.00	41.04	
ATOM ATOM	2766	OH2	TIP3		-2.328	-3.576	11.086	1.00	44.89	
ATOM	2769	OH2	TIP3		34.919	-4.069	19.070	1.00	53.72	
ATOM	2772	OH2	TIP3		80.124	17.865	9.324	1.00	28.96	
ATOM	2775	OH2	TIP3	32	5.417	3.492	10.771	1.00	34.07	

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ATOM	2778	OH2	TIP3	33	-10.718	4.889	11.542	1.00	30.81
MOTA	2781	OH2	TIP3	34	29.486	-8.823	20.599	1.00	51.35
MOTA	2784	OH2	TIP3	35	6.151	3.065	13.821	1.00	34.56
ATOM	2787	OH2	TIP3	36	31.907	2.919	0.361	1.00	48.13
MOTA	2790	OH2	TIP3	37	19.974	1.928	-3.873	1.00	30.12
MOTA	2793	OH2	TIP3	38	61.976	2.660	32.604	1.00	36.01
MOTA	2796	OH2	TIP3	39	21.084	-7.119	-3.759	1.00	20.12
ATOM	2799	OH2	TIP3	40	-15.729	8.693	22.468	1.00	54.88
ATOM	2802	OH2	TIP3	41	40.160	2.461	8.734	1.00	37.95
ATOM	2805	OH2	TIP3	42	19.248	11.349	0.190	1.00	37.63
MOTA	2808	OH2	TIP3	43	66.856	9.143	17.185	1.00	27.91
ATOM	2811	OH2	TIP3	44	87.262	19.150	18.734	1.00	57.83
MOTA	2814	OH2	TIP3	45	74.597	17.144	3.987	1.00	42.19
MOTA	2817	OH2	TIP3	46	29.192	16.988	10.582	1.00	37.28
MOTA	2820	OH2	TIP3	47	66.415	7.073	14.829	1.00	34.86
MOTA	2823	OH2	TIP3	48	85.063	21.453	5.510	1.00	27.42
MOTA	2826	ЭН2	TIP3	49	-4.716	2.835	2.998	1.00	40.54
ATOM	2829	OH2	TIP3	50	19.369	5.069	4.888	1.00	38.40
MOTA	2832	OH2	TIP3	51	34.750	5.517	24.999	1.00	29.11
ATOM	2835	OH2	TIP3	52	34.740	-16.765	14.093	1.00	32.68
MOTA	2838	OH2	TIP3	53	59.994	7.555	27.844	1.00	32.60
ATOM	2841	OH2	TIP3		-7.401	-1.595	6.080	1.00	43.73
ATOM	2844	OH2	TIP3	55	55.257	12.084	25.108	1.00	44.32
ATOM	2847	OH2	TIP3	56	68.239	6.953	16.647	1.00	44.46
ATOM	2850	OH2	TIP3	57	73.621	20.852	18.820	1.00	29.47
MOTA	2853	OH2	TIP3	58	3.399	-3.294	-8.210	1.00	22.31
ATOM	2856	ОН2 ОН2	TIP3	60	37.999	10.824	5.505	1.00	31.62 40.76
MOTA MOTA	2859 2862	OH2	TIP3 TIP3	61	29.779 49.114	-9.515 1.432	-1.395 12.261	1.00	29.92
ATOM	2865	OH2	TIP3	62	41.257	4.012	29.005	1.00	39.24
ATOM	2868	OH2	TIP3	63	11.113	-12.848	1.296	1.00	34.36
ATOM	2871	OH2	TIP3	64	-1.221	-4.593	21.504	1.00	34.24
ATOM	2874	OH2	TIP3		30.002	16.453	13.258	1.00	49.66
ATOM	2877	OH2	TIP3	66	8.212	4.106	3.434	1.00	36.54
ATOM	2880	OH2	TIP3	67	72.868	18.807	22.589	1.00	38.26
MOTA	2883	OH2	TIP3	68	-8.056	-3.666	25.021	1.00	39.81
ATOM	2886	OH2	TIP3	69	66.436	-4.683	28.008	1.00	60.97
MOTA	2889	OH2	TIP3	70	22.063	-20.641	4.804	1.00	42.25
MOTA	2892	OH2	TIP3	71	59.860	-7.407	4.859	1.00	56.78
MOTA	2895	OH2	TIP3	72	16.887	-13.832	-2.611	1.00	59.32
ATOM	2898	OH2	TIP3	73	-15.108	7.351	4.303	1.00	31.87
MOTA	2901	OH2	TIP3	74	32.901	2.922	13.663	1.00	37.89
ATOM	2904	OH2	TIP3	75	0.173	-2.666	11.035	1.00	39.12
ATOM	2907	OH2	TIP3	76	17.533	2.317	5.808	1.00	18.66
ATOM	2910	OH2	TIP3	77	27.183	3.730	6.349	1.00	29.04
ATOM	2913	OH2	TIP3	78	-8.812	5.887	9.703	1.00	30.53
ATOM	2916	OH2	TIP3	79	1.614	-2.195	8.694	1.00	30.79
MOTA	2919	ОН2	TIP3	80	-5.304	-3.157	6.846	1.00	47.38
MOTA	2922	OH2	TIP3		17.401	2.918	1.973	1.00	20.47
ATOM	2925	OH2	TIP3		20.333	3.188	3.159	1.00	24.44
MOTA	2928	OH2	TIP3		0.408	-2.516	22.276	1.00	31.11
ATOM	2931	OH2	TIP3		20.095	-6.123	-1.372	1.00	17.62
ATOM	2934	OH2	TIP3		11.018	-15.627	7.421	1.00	60.29
MOTA	2937	OH2	TIP3	86	4.089	-12.037	11.797	1.00	39.47

MOTA	2940	OH2	TIP3	87	6.459	0.908	-3.278	1.00	30.31
ATOM	2943	OH2	TIP3	88	-13.493	1.004	5.319	1.00	41.13
MOTA	2946	OH2	TIP3	89	15.418	-7.532	0.022	1.00	21.29
MOTA	2949	OH2	TIP3	90	-2.128	-5.834	4.052	1.00	57.55
MOTA	2952	OH2	TIP3	91	12.731	4.833	-4.212	1.00	44.52
MOTA	2955	OH2	TIP3	92	69.320	27.812	2.191	1.00	37.47
ATOM	2958	OH2	TIP3	93	24.851	-12.871	0.285	1.00	44.73
ATOM	2961	OH2	TIP3	94	60.301	-4.459	33.927	1.00	40.13
MOTA	2964	C:H2	TIP3	95	10.488	5.951	3.205	1.00	41.53
MOTA	2967	OH2	TIP3	96.	-9.708	-4.233	4.439	1.00	29.77
MOTA	2970	OH2	TIP3	97	72.950	-1.768	10.144	1.00	39.69
MOTA	2973	OH2	TIP3	98	-3.287	5.612	30.618	1.00	34.65
MOTA	2976	OH2	TIP3	99	36.658	1.007	11.717	1.00	35.43
ATOM	29.79	OH2	TIP3	100	21.221	6.459	16.863	1.00	20.70
ATOM	2982	OH2	TIP3	101	5.833	-8.726	22.274	1.00	47.13
MOTA	2985	OH2	TIP3	102	-13.529	7.868	17.445	1.00	31.95
ATOM	2988	OH2	TIP3	103	26.795	-10.682	-0.807	1.00	28.65
MOTA	2991	OH2	TIP3	104	23.711	1.909	18.309	1.00	28.29
MOTA	2994	OH2	TIP3	105	-2.187	12.232	3.920	1.00	44.98
ATOM.	2997	OH2	TIP3	106	59.483	12.398	33.535	1.00	39.58
MOTA	3000	OH2	TIP3	107	4.439	-10.915	1.996	1.00	43.77
ATOM	3003	OH2	TIP3	108	8.041	2.687	6.648	1.00	45.32
ATOM	3006	OH2	TIP3	109	75.836	1.477	25.476	1.00	41.65
ATOM	3009	OH2	TIP3	110	48.604	15.594	14.349	1.00	36.36
ATOM	3012	OH2	TIP3	111	2.396	11.387	9.259	1.00	34.21
ATOM	3015	OH2	TIP3	112	82.927	26.453	12.907	1.00	36.54
ATOM	3018	OH2	TIP3	113	8.983	-6.631	-3.299	1.00	47.01
MOTA	3021	OH2		114	-8.690	4.367	4.504	1.00	41.25
MOTA	3024	OH2	TIP3		7.941	-13.921	8.777	1.00	36.12
ATOM	3027	OH2	TIP3		51.295	6.440	10.632	1.00	28.37
MOTA	3030	OH2	TIP3		20.432	3.771	15.637	1.00	31.22
MOTA	3033	OH2		118	72.882	3.887	20.227	1.00	30.22
ATOM	3036	OH2	TIP3		5.187	-11.863	22.711	1.00	47.49
MOTA	3039	OH2	TIP3		33.889	2.571	16.293	1.00	40.04
ATOM	3042	OH2		121	9.504	-12.183	7.160	1.00	31.48
ATOM	3045	OH2		122	8.397	3.827	-1.647	1.00	46.92
ATOM	3048	OH2	TIP3		7.281	7.321	2.391	1.00	62.46
ATOM	3051	OH2	TIP3		35.682	-1.725	0.534	1.00	36.75
ATOM	3054	OH2		125	44.465	10.095	11.089	1.00	44.72
ATOM	3057	OH2	TIP3		45.247	11.893	21.405	1.00	33.51
MOTA	3060	OH2	TIP3		57.386	-10.506	14.020	1.00	45.72
ATOM	3063	OH2	TIP3		-3.033	15.103	16.644	1.00	38.48
MOTA	3066	OH2		129	85.621	11.111	8.814	1.00	38.13
ATOM	3069	OH2		130	13.040	-2.760	2.176	1.00	31.26
ATOM	3072	OH2		131	75.607	3.932	20.836	1.00	55.09
MOTA	3075	OH2		132	13.080	7.467	-2.358	1.00	35.05
ATOM	3078	OH2		133	11.308	-9.967	0.995	1.00	28.96
MOTA	3081	OH2		134	13.716	-16.170	3.848	1.00	44.64
ATOM	3084	OH2		135	-6.498	-3.706	16.178	1.00	43.17
MOTA	3087	OH2		136	25.841	-12.949	3.950	1.00	41.14
ATOM	3090	OH2		137	-16.285	10.803	6.585	1.00	45.75
ATOM	3093	OH2		138	86.457	12.585	6.477	1.00	36.37
ATOM	3096	OH2		139	32.097	-4.644	2.224	1.00	28.35
MOTA	3099	OH2	TIP3	140	44.936	7.528	11.961	1.00	46.60

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ATOM 3102 OH2 TIP3 141 80.781 16.353 12.162 1.00 41.46 MOTA 3105 OH2 TIP3 142 2.547 -7.532 -1.453 1.00 41.42 ATOM 3108 OH2 TIP3 143 31.850 -5.907 21.194 1.00 54.70 **ATOM** 3111 OH2 TIP3 144 74.524 -2.663 12.264 1.00 40.35 **ATOM** 3114 OH2 TIP3 145 7.592 6.769 -0.931 1.00 58.34 **ATOM** 3117 OH2 TIP3 146 71.168 5.735 21.648 1.00 27.86 **ATOM** 3120 OH2 TIP3 147 67.876 -4.900 8.725 1.00 33.58 **ATOM** 3123 OH2 TIP3 148 0.554 -10.181 6.605 1.00 75.65 ATOM 3126 OH2 TIP3 149 67.965 18.266 10.874 1.00 30.42 **ATOM** 3129 OH2 TIP3 150 3.509 8.125 4.021 1.00 40.77 MOTA 3132 TIP3 151 OH2 52.216 12.175 18.131 1.00 47.63 **MOTA** 3135 OH2 TIP3 152 -10.336 6.394 5.014 1.00 48.53 **ATOM** 3138 OH2 TIP3 153 76.427 1.384 1.00 -1.196 47.21 **ATOM** 3141 OH2 TIP3 154 70.16 10.116 -12.199 17.089 1.00 **ATOM** 3144 OH2 TIP3 155 34.043 14.595 18.314 1.00 40.56 **ATOM** 3147 OH2 TIP3 156 2.488 -8.304 16.835 1.00 64.47 ATOM 3150 OH2 TIP3 157 29.610 1.954 6.685 1.00 48.74 ATOM 3153 OH2 TIP3 158 32.578 -17.270 12.109 1.00 37.35 MOTA 3156 OH2 TIP3 159 42.013 18.106 11.196 1.00 68.33 MOTA 3159 OH2 TIP3 160 87.646 10.346 5.465 1.00 75.39 **ATOM** 3162 OH2 TIP3 161 69.931 -3.739 24.921 1.00 70.42 **ATOM** 3165 OH2 TIP3 162 77.277 5.700 23.531 1.00 53.26 **ATOM** 3168 OH2 TIP3 163 34.172 15.704 1.865 1.00 44.88 ATOM 3171 OH2 TIP3 164 -9.871 7.514 7.751 1.00 39.18 **ATOM** 3174 OH2 TIP3 165 11.814 5.604 7.443 1.00 46.70 3177 **ATOM** OH2 TIP3 166 -8.801 13.912 13.532 1.00 52.89 MOTA 3180 OH2 TIP3 167 32.195 3.409 18.336 1.00 32.33 MOTA 3183 OH2 TIP3 168 -8.858 9.696 24.279 1.00 38.90 **ATOM** 3186 OH2 TIP3 169 -1.135 -6.924 15.691 1.00 43.05 **ATOM** 3189 OH2 TIP3 170 79.806 0.323 15.371 1.60 36.91 ATOM 3192 OH2 TIP3 171 67.181 20.622 -1.545 1.00 44.72 **MOTA** 3195 OH2 TIP3 172 -0.823 3.732 1.065 1.00 52.11 **ATOM** 3198 OH2 TIP3 173 -0.130 6.021 2.491 1.00 40.87 MOTA 3201 OH2 TIP3 174 -1.027 8.941 1.064 1.00 60.72 MOTA 3204 OH2 TIP3 175 -5.566 8.867 2.163 1.00 47.25 MOTA 3207 OH2 TIP3 176 -7.259 10.294 4.033 1.00 53.61 MOTA 3210 OH2 TIP3 177 2.664 7.247 1.058 1.00 46.41 MOTA 3213 OH2 TIP3 178 5.295 10.728 8.257 1.00 39.84 MOTA 3216 OH2 TIP3 179 63.743 12.726 22.713 1.00 49.55 **ATOM** 3219 OH2 TIP3 180 79.165 17.948 1.016 1.00 51.41 MOTA 3222 OH2 TIP3 181 13.823 -1.538 -3.942 1.00 39.85 **ATOM** 3225 OH2 TIP3 182 59.255 3.213 32.873 1.00 76.77 MOTA 3228 OH2 TIP3 183 32.210 13.612 20.027 1.00 60.41 MOTA 3231 OH2 TIP3 184 72.606 16.267 22.574 1.00 60.78 MOTA 3234 OH2 TIP3 185 -0.147 5.713 30.877 1.00 50.19 MOTA 3237 OH2 TIP3 186 -1.207 -4.507 27.969 1.00 65.19 ATOM 3240 OH2 TIP3 187 81.340 15.584 16.808 1.00 64.48 **ATOM** 3243 OH2 TIP3 188 -17.535 3.884 23.785 1.00 57.17 **ATOM** 3246 OH2 TIP3 189 27.503 10.697 14.669 1.00 36.11 MOTA 3249 OH2 TIP3 190 34.585 4.535 27.618 1.00 61.68 **MOTA** 3252 OH2 TIP3 191 -3.701 -4.982 9.069 1.00 43.66 MOTA 3255 OH2 TIP3 192 42.524 7.811 22.390 1.00 34.53 **ATOM** 3258 OH2 TIP3 193 52.937 11.764 21.790 1.00 36.19 MOTA 3261 OH2 TIP3 194 -7.665 8.600 6.358 1.00 59.08

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ATOM	3264	OH2	TIP3	· 195	86.880	5.187	16.579	1.00	55.88			
ATOM	3267	OH2	TIP3	196	55.377	16.147	20.540	1.00	48.25			
ATOM	3270	OH2	TIP3	197	51.394	19.664	22.988	1.00	46.81			
ATOM	3273	OH2	TIP3	198	20.021	7.087	7.226	1.00	52.98		•	
MOTA	3276	ОН2	TIP3	199	28.959	1.819	-3.219	1.00	40.50			
ATOM	3279	OH2	TIP3	200	26.533	2.812	-4.295	1.00	54.24		_	
ATOM	3282	OH2	TIP3	201	36.739	3.003	18.397	1.00	42.13			
ATOM	3285	OH2	TIP3	202	16.968	-20.752	14.318	1.00	54.54			
ATOM	3288	OH2	TIP3	203	28.177	-14.418	6.134	1.00	61.36			
ATOM	3291	OH2	TIP3	204	31.488	1.501	-1.796	1.00	47.49			
ATOM	3294	OH2	TIP3	205	10.665	-16.494	15.731	1.00	41.42		-	
MOTA	3297	OH2	TIP3	206	6.916	-12.200	6.160	1.00	61.94			
ATOM	3300	OH2	TIP3	207	-12.659	14.357	10.908	1.00	52.96			
ATOM	3303	OH2	TIP3	208	11.274	9.662	-1.588	1.00	48.45	 		
MOTA	3306	OH2	TIP3	209	11.491	12.484	-1.531	1.00	44.51			
MOTA	3309	OH2	TIP3	210	34.037	13.520	-1.011	1.00	48.43			
MOTA	3312	OH2	TIP3	211	31.162	18.259	7.980	1.00	44.86			
MOTA	3315	OH2	TIP3	212	36.937	11.633	-1.971	1.00	49.85			
MOTA	3318	OH2	TIP3	213	64.024	13.599	26.505	1.00	37.53			
ATOM	3321	OH2	TIP3	214	36.528	5.933	14.857	1.00	57.04			
ATOM	3324	OH2	TIP3	215	90.599	4.042	6.342	1.00	54.08			
MOTA	3327	OH2	TIP3	216	50.139	-11.645	10.526	1.00	54.64			
ATOM	3330	OH2	TIP3	217	66.523	-1.024	30.536	1.00	39.41			
ATOM	3333	OH2	TIP3	218	74.880	18.976	20.591	1.00	41.84			
ATOM	3336	OH2	TIP3	219	-3.095	9.744	3.142	1.00	52.35			
MOTA	3339	OH2	TIP3	220	5.601	-3.682	25.022	1.00	29.30			
ATOM	3342	OH2	TIP3		35.616	6.407	12.455	1.00	44.48			
ATOM	3345	OH2	TIP3		-5.381	16.006	14.081	1.00	44.23			
MOTA	3348	OH2	TIP3		46.509	-11.503	26.814	1.00	53.82			
ATOM	3351	OH2	TIP3		-3.791	-5.481	20.929	1.00	61.42			
ATOM	3354	OH2	TIP3		1.622	-3.876	-0.402	1.00	58.60			
MOTA	3357	OH2	TIP3		86.244	11.220	23.133	1.00	59.84			
MOTA	3360	OH2	TIP3		11.011	7.959	5.659	1.00	63.07			
ATOM	3363	OH2	TIP3		64.610	-8.031	20.406	1.00	48.11			
ATOM	3366	OH2	TIP3		11.446	-17.829	13.438	1.00	51.35			
ATOM	3369	OH2	TIP3		72.056	1.258	-1.830	1.00	43.88			
ATOM	3372	OH2	TIP3		57.359	9.732	11.744	1.00	65.45			
ATOM	3375	OH2	TIP3			20.728	30.066	1.00	61.52			
ATOM	3378	OH2	TIP3		66.723	16.772	15.661	1.00	43.79			
ATOM	3381	OH2	TIP3		88.036	22.036	4.257	1.00	61.83			
ATOM	3384	OH2	TIP3		12.085	2.346	27.862	1.00	46.29			
ATOM	3387	OH2	TIP3		64.898	-0.425	3.209	1.00	50.06			
ATOM	3390	OH2	TIP3		72.114	28.348	7.731	1.00	53.01			
MOTA	3393	OH2	TIP3		25.792	-8.081	27.181	1.00	55.19			
ATOM	3396	OH2	TIP3		-18.262	10.614	12.607	1.00	51.54			
ATOM	3399	OH2	TIP3	-	30.336	11.280	16.201	1.00	46.53			
ATOM	3402	OH2	TIP3		22.712	-15.818	-2.226	1.00	47.29			
ATOM	3405	OH2	TIP3		29.700	9.496	18.074	1.00	40.10			
ATOM	3408	OH2	TIP3		63.297	-0.480	5.497	1.00	49.90		-	
ATOM	3411	OH2	TIP3		61.458	7.093	11.497	1.00	45.71			
ATOM	3414	OH2	TIP3		-0.217	2.232	32.172	1.00	46.12			
ATOM	3417	OH2	TIP3	246	66.196	6.250	12.159	1.00	34.47		•	

TABLE 3

			•							
Atom		tom	A.A		x	Y	Z	OCC	В	
No.		уре	Тур							
ATOM	1	N	GLU	1464	-13.712	16.996	8.424		61.15	_
MOTA	3	CA	GLU	1464	-12.478	17.133	7.646	1.00	60.03	
MOTA	4	CB	GLU	1464	-11.465	18.020	8.378	1.00	62.43	
MOTA	5	C	GLU	1464	-11.865	15.766	7.319		57.36	
ATOM	6	0	GLU	1464	-11.765	15.402	6.145		60.80	
ATOM	. 7	N	LEU	1465	-11.466	15.003	8.333		50.25	
ATOM	9	CA	LEU	1465	-10.899	13.691	8.067	1.00	42.73	
MOTA	10	CB	LEU	1465	-10.097	13.171	9.258	1.00	41.34	
ATOM	11	CG	LEU	1465	-8.571	13.277	9.169	1.00	39.78	
ATOM	12		LEU	1465	-8.175	14.728	8.977		45.14	
ATOM	13		LEU	1465	-7.926	12.722	10.426		34.20	-
MOTA	14	C	LEU	1465	-12.009	12.706	7.748		39.42	
ATOM	15	0	LEU	1465	-13.070	12.719	8.375		36.63	
ATOM	16	Ŋ	PRO	1466	-11.821	11.919	6.682		38.54	
ATOM ATOM	17	CD	PRO	1466	~10.682	12.019	5.751		37.04	
	18	CA	PRO	1466	-12.781	10.902	6.232		38.75	
ATOM ATOM	1.9	CB	PRO	1466	-12.176	10.426	4.910		39.49	
ATOM	20	CG	PRO	1466	-10.681	10.667	5.109		40.64	
ATOM	21 22	C C	PRO	1466	-12.859	9.756	7.246		39.08	
ATOM	23	N	PRO GLU	1466 1467	-11.834	9.283	7.748		41.23	
ATOM	25	CA	GLU	1467	-14.064 -14.247	9.278	7.513		37.11	
ATOM	26	CB	GLU	1467		8.213 8.123	8.482 8.863		35.96	
ATOM	27	CG	GLU	1467	-15.725 -16.334	9.410			39.90	
ATOM	28	CD	GLU	1467	-17.823	9.280	9.417 9.694	1.00		
ATOM	29		GLU	1467	-18.294	8.135	9.854		51.50	
ATOM	30		GLU	1467	-18.529	10.315	9.756	1.00 1.00		
ATOM	31	C	GLU	1467	-13.794	6.865	7.939	1.00		
ATOM	32	0	GLU	1467	-13.885	6.632	6.740	1.00		
MOTA	33	N	ASP	1468	-13.291	5.991	8.813	1.00		
MOTA	35	CA	ASP	1468	-12.869	4.649	8.409	1.00		
ATOM	36	СВ	ASP	1468	-11.362	4.567	8.120	1.00		
ATOM	37	CG	ASP	1468	-10.942	3.223	7.507	1.00		
ATOM	38	OD1	ASP	1468	-11.689	2.225	7.592	1.00		
ATOM	39	OD2		1468	-9.836	3.165	6.935	1.00		
ATOM	40	С	ASP	1468	-13.244	3.672	9.512	1.00		
ATOM	41	0	ASP	1468	-12.462	3.404	10.437	1.00		
MOTA	42	N	PRO	1469	-14.446	3.089	9.403	1.00		
ATOM	43	CD	PRO	1469	-15.401	3.311	8.298	1.00		
ATOM	44	CA	PRO	1469	-14.981	2.124	10.365	1.00		
MOTA	45	CB	PRO	1469	-16.235	1.615	9.659	1.00		
MOTA	46	CG	PRO	1469	-16.690	2.811	8.879	1.00		
MOTA	47	С	PRO	1469	-14.029	0.974	10.687	1.00		
MOTA	48	0	PRO	1469	-14.136	0.364	11.748	1.00		
MOTA	49	N	ARG	1470	-13.128	0.666	9.758	1.00		
ATOM	51	CA	ARG	1470	-12.161	-0.414	9.947	1.00		

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ATOM	52	CB	ARG	1470	-11.363	-0.661	8.666	1.00 27.12
ATOM	53	CG	ARG	1470	-12.150	-1.014	7.424	1.00 29.72
MOTA	54	CD	ARG	1470	-11.189	-1.184	6.236	1.00 30.37
MOTA	55	NE	ARG	1470	-10.450	0.044	5.971	1.00 32.56
MOTA	57	CZ	ARG	1470	-9.624	0.211	4.948	1.00 37.69
MOTA	58		ARG	1470	-9.428	-0.784	4.091	1.00 44.25
ATOM	61	NH2	ARG	1470	-8.997	1.370	4.778	1.00 34.12
ATOM	64	С	ARG	1470	-11.129	-0.176	11.051	1.00 27.58
ATOM	65	0	ARG	1470	-10.504	-1.123	11.522	1.00 28.12
MOTA	66	N	TRP	1471	-10.900	1.079	11.421	1.00 27.62
MOTA	68	CA	TRP	1471	-9.870	1.362	12.408	1.00 26.66
MOTA	69	CB	TRP	1471	-8.661	1.938	11.686	1.00 24.95
ATOM	70	CG	TRP	1471	-8.010	0.951	10.790	1.00 25.65
ATOM	71	CD2	TRP	1471	-7.100	-0.083	11.186	1.00 23.19
ATOM	72	CE2	TRP	1471	-6.734	-0.776	10.022	1.00 21.80
ATOM	73	CE3	TRP	1471	-6.567	-0.489	12.414	1.00 21.84
ATOM	74	CD1	TRP	1471	-8.155	0.843	9.435	1.00 23.15
ATOM	75	NE1	TRP	1471	-7.388	-0.192	8.970	1.00 23.32
ATOM	77	CZ2	TRP	1471	-5.855	-1.857	10.052	1.00 22.54
ATOM	78	CZ3	TRP	1471	-5.698	-1.564	12.439	1.00 21.72
ATOM	79	CH2	TRP	1471	~5.352	-2.235	11.269	1.00 21.90
ATOM	80	С	TRP	1471	-10.224	2.278	13.558	1.00 28.44
ATOM	81	0	TRP	1471	-9.497	2.334	14.546	1.00 29.29
MOTA	82	N	GLU	1472	-11.317	3.015	13.424	1.00 29.49
ATOM	84	CA	GLU	1472	-11.719	3.962	14.453	1.00 29.97
ATOM	85	CB	GLU	1472	-12.920	4.769	13.961	1.00 33.30
ATOM	86	CG	GLU	1472	-13.218	6.050	14.731	1.00 33.27
MOTA	87	CD	GLU	1472	-12.475	7.249	14.195	1.00 34.26
ATOM	88	OE1	GLU	1472	-11.970	7.191	13.055	1.00 38.00
ATOM	89	OE2	GLU	1472	-12.413	8.265	14.910	1.00 34.01
ATOM	90	С	GLU	1472	-12.034	3.366	15.826	1.00 27.30
ATOM	91	0	GLU	1472	-12.640	2.309	15.945	1.00 28.36
ATOM	92	N	LEU	1473	-11.619	4.069	16.866	1.00 25.91
ATOM	94	CA	LEU	1473	-11.896	3.652	18.229	1.00 24.89
ATOM	95	СВ	LEU	1473	-10.625	3.210	18.948	1.00 24.70
ATOM	96	CG	LEU	1473	-10.766	2.923	20.454	1.00 24.56
ATOM	97	CD1	LEU	1473	-11.498	1.613	20.701	1.00 21.89
ATOM	98	CD2		1473	-9.385	2.872	21.095	1.00 23.90
ATOM	99	С	LEU	1473	-12.426	4.907	18.882	1.00 27.05
ATOM	100	0	LEU	1473	-11.968	6.016	18.567	1.00 25.17
ATOM	101	N	PRO	1474	-13.479	4.766	19.706	1.00 28.20
ATOM	102	CD	PRO	1474	-14.290	3.551	19.886	1.00 29.92
ATOM	103	CA	PRO	1474	-14.088	5.897	20.411	1.00 20.52
ATOM	104	СВ	PRO	1474	-15.197	5.224	21.226	1.00 30.01
ATOM	105	CG	PRO	1474	-15.613	4.110	20.357	1.00 24.28
ATOM	106	c	PRO	1474	-13.036	6.545	20.337	1.00 24.28
ATOM	107	0	PRO	1474	-12.253	5.838	21.312	1.00 32.98
ATOM	108	N	ARG	1475	-13.035	7.875	21.366	1.00 34.79
ATOM	110	CA	ARG	1475	-12.060	8.606	22.168	1.00 32.75
ATOM	111	CB	ARG	1475	-12.060			
ATOM	112	CG	ARG	1475	-12.250	10.116	21.997	1.00 34.21
ATOM						10.549	20.559	1.00 42.48
AT ON	113	CD	ARG	1475	-11.956	12.056	20.364	1.00 45.16

ATOM	114	NE	ARG	1475	-11.655	12.317	18.954	1.00 45.65
MOTA	116	CZ	ARG	1475	-10.447	12.599	18.484	1.00 41.31
ATOM	117	NH1	ARG	1475	-9.420	12.686	19.318	1.00 35.94
ATOM	120	NH2	ARG	1475	-10.253	12.673	17.172	1.00 42.37
MOTA	123	C	ARG	1475	-12.114	8.232	23.641	1.00 35.29
MOTA	124	0	ARG	1475	-11.094	8.178	24.318	1.00 37.28
ATOM	125	N	ASP	1476	-13.304	7.931	24.129	1.00 35.37
ATOM	127	CA	ASP	1476	-13.468	7.570	25.526	1.00 36.97
ATOM	128	CB	ASP	1476	-14.952	7.586	25.896	1.00 39.47
ATOM	129	CG	ASP	1476	-15.748	6.501	25.205	1.00 40.02
ATOM	130	OD1	ASP	1476	-15.221	5.809	24.320	1.00 41.08
ATOM	131	OD2	ASP	1476	-16.926	6.327	25.571	1.00 47.00
ATOM	132	С	ASP	1476	-12.850	6.225	25.894	.1.00 36.07
ATOM	133	0	ASP	1476	-12 830	5.842	27.066	1.00 36.26
ATOM	134	N	ARG	1477	-12.382	5.495	24.888	1.00 36.94
MOTA	136	CA	ARG	1477	-11.766	4.189	25.101	1.00 35.22
MOTA	137	CB	ARG	1477	-12.081	3.268	23.925	1.00 34.29
ATOM	138	CG	ARG	1477	-13.546	3.056	23.675	1.00 32.23
ATOM	139	CD	ARG	1477	-14.206	2.434	24.879	1.00 30.56
ATOM	140	NE	ARG	1477	-14.426	3.419	25.925	1.00 31.86
ATOM	142	CZ	ARG	1477	-14.730	3.126	27.182	1.90 33.09
ATOM	143	NH1	ARG	1477	-14.855	1.858	27.563	1.00 35.00
ATOM	146	NH2	ARG	1477	-14.904	4.101	28.053	1.00 29.62
ATOM	149	C	ARG	1477	-10.262	4.270	25.271	1.00 35.51
ATOM	1.50	0	ARG	1477	-9.621	3.290	25.637	1.00 35.44
ATOM	151	N	LEU	1478	-9.704	5.444	25.023	1.00 34.59
ATOM	i53	CA	LEU	1478	-8.270	5.630	25.129	1.00 36.35
ATOM	154	CB	LEU	1478	-7.750	6.254	23.840	1.00 36.41
ATOM	155	CG	LEU	1478	-6.250	6.185	23.556	1.00 37.19
ATOM	156		LEU	1478	-5.791	4.728	23.479	1.00 34.63
MOTA	157		LEU	1478	-5.959	6.914	22.251	1 00 34.88
ATOM	158	С	LEU	1478	-7.901	6.517	26.325	1.00 38.74
MOTA	159	0	LEU	1478	-8.146	7.733	26.309	1.00 41.20
ATOM	160	N	VAL	1479	-7.311	5.907	27.355	1.00 36.92
ATOM	162	CA	VAL	1479	-6.885	6.622	28.560	1.00 35.79
ATOM	163	СВ	VAL	1479	-6.929	5.693	29.780	1.60 35.81
ATOM	164		VAL	1479	-6.579	6.453	31.032	1.00 40.11
ATOM	165		VAL	1479	-8.302	5.056	29.907	1.00 35.59
MOTA	166	С	VAL	1479	-5.438	7.118	28.362	1.00 36.60
ATOM	167	0	VAL	1479	-4.479	6.369	28.583	1.00 33.48
ATOM	168	N	LEU	1480	-5.282	8.372	27.938	1.00 39.09
ATOM	170	CA	LEU	1480	-3.949	8.932	27.675	1.00 42.05
ATOM	171	CB	LEU	1480	-4.040	10.277	26.952	1.00 41.08
ATOM	172	CG	LEU	1480	-4.633	10.286	25.529	1.00 39.28
ATOM	173		LEU	1480	-4.766	11.720	25.051	1.00 40.04
ATOM	174	CD2		1480	-3.758	9.489	24.582	1.00 39.66
ATOM	175	C	LEU	1480	-3.001	9.027	28.867	1.00 41.51
ATOM	176	0	LEU	1480	-3.312	9.637	29.886	1.00 41.73
ATOM	177	N	GLY	1481	-1.817	8.444	28.697	1.00 40.68
ATOM	179	CA	GLY	1481	-0.849	8.439	29.775	1.00 41.28
ATOM	180	C	GLY	1481	0.412	9.225	29.529	1.00 43.08
ATOM	181	0	GLY	1481	0.474	10.147	28.701	1.00 45.65

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ATOM	182	N	LYS	1482	1.481	8.825	30.219	1.00 42.54
ATOM	184	CA	LYS	1482	2.781	9.453	30.128	1.00 43.74
MOTA	185	CB	LYS	1482	3.670	8 842	31.229	1.00 46.34
MOTA	186	CG	LYS	1482	5.155	8.979	30.954	1.00 52.23
MOTA	187	CD	LYS	1482	5.867	7.716	31.382	1.00 56.63
ATOM	188	CE	LYS	1482	5.373	6.518	30.607	1.00 54.20
MOTA	189	NZ	LYS	1482	6.199	5.320	30.955	1.00 59.97
ATOM	193	C	LYS	1482	3.552	9.422	28.806	1.00 43.96
ATOM	194	0	LYS	1482	3.557	8.422	28.111	1.00 44.68
ATOM	195	N	PRO	1483	4.259	10.521	28.481	1.00 44.06
ATOM	196	CD	PRO	1483	4.339	11.798	29.208	1.00 43.53
ATOM	197	CA	PRO	1483	5.005	10.573	27.208	1.00 44.07
ATOM	-198 -	· CB	-PRO	1483	5.590	12.004	27.281	
ATOM	199	CG	PRO	1483	4.630	12.738	28.114	1.00 43.75
ATOM	200	С	PRO	1483	6.172	9.543	27.116	1.00 43.47
ATOM	201	0	PRO	1483	6.853	9.308	28.120	1.00 43.47
ATOM	202	N	LEU	1484	6.408	9.001	25.932	1.00 41.71
ATOM	204	CA	LEU	1484	7.512	8.045	25.663	1.00 38.05
MOTA	205	СВ	LEU	1494	6.964	6.803	24.927	1.00 33.38
ATOM	206	CG	LEU	1484	5.001	5.992	25.770	1.00 31.95
ATOM	207		LEU	1484	5.258	4.914	24.975	1.00 27.41
ATOM	208		LEU	1464	6.750	5.396	26.953	1.60 29.64
ATOM	209	C	LEU	1484	8.603	8.710	24.855	1.00 40.09
ATOM	210	O	LEU	1484	8.334	9.499	23.960	1.00 41.74
ATOM	211	N	GLY	1485	9.843	8.387	25.197	1.00 43.19
ATOM	213	CA	GLY	1485	10.976	8.923	24.512	1.00 50.32
ATOM	214	С	GLY	1485	11.261	10.408	24.697	1.00 54.65
ATOM	215	o	GLY	1485	11.036	10.973	25.770	1.00 54.73
ATOM	216	N	GLU	1486	11.747	11.072	23.647	1.00 59.07
ATOM	218	CA	GLU	1486	12.081	12.483	23.666	1.00 61.01
ATOM	219	CB	GLU	1486	13.489	12.646	24.275	1.00 62.51
MOTA	220	C	GLU	1486	12.014	13:183	22.295	1.00 62.48
MOTA	221	0	GLU	1486	12.901	13.970	21.949	1.00 64.10
ATOM	222	N	GLY	1487	10.975	12.892	21.519	1.00 62.29
ATOM	224	C.A	GLY	1487	10.792	13.522	20.236	1.00 59.87
MOTA	225	C	GLY	1487	11.469	12.881	19.044	1.00 58.88
ATOM	226	0	GLY	1487	11.447	13.426	17.950	1.00 60.19
ATOM	227	N	ALA	1488	12.073	11.714	19.239	1.00 57.19
ATOM	229	CA	ALA	1488	12.721	11.016	18.140	1.00 55.59
ATOM	230	CB	ALA	1488	13.477	9.804	18.663	1.00 56.35
ATOM	231	C	ALA	1488	11.690	10.601	17.112	1.00 54.96
ATOM	232	0	ALA	1488	11.927	10.626	15.913	1.00 56.42
ATOM	233	N	PHE	1489	10.509	10.241	17.598	1.00 54.99
ATOM	235	CA	PHE	1489	9.401	9.807	16.721	1.00 54.07
ATOM	236	CB	PHE	1489	8.857	8.454	17.162	1.00 51.18
MOTA	237	CG	PHE	1489	9.880	7.373	17.137	1.00 46.81
ATOM	238	CD1	PHE	1489	10.641	7.093	18.271	1.00 46.81
MOTA	239	CD2	PHE	1489	10.096	6.612	15.984	1.00 48.30
MOTA	240	CE1	PHE	1489	11.585	6.090	18.262	1.00 47.41
MOTA	241	CE2		1489	11.040	5.601	15.963	1.00 48.23
ATOM	242	CZ	PHE	1489	11.794	5.336	17.111	1.00 47.94
ATOM	243	С	PHE	1489	8.261	10.814	16.748	1.00 54.90
					- · · · ·			00 34.90

MOTA	244	0	PHE	1489	7.199	10.565	16.184	1.00 59.10
MOTA	245	N	GLY	1490	8.431	11.908	17.504	1.00 53.55
ATOM	247	CA	GLY	1490	7.432	12.958	17.611	1.00 50.20
ATOM	248	С	GLY	1490	6.745	12.844	18.942	1.00 49.82
MOTA	249	0	GLY	1490	7.266	12.161	19.837	1.00 50.95
MOTA	250	N	GLN	1491	5.614	13.514	19.124	1.00 49.53
ATOM	252	CA	GLN	1491	4.922	13.441	20.395	1.00 49.16
ATOM	253	CB	GLN	1491	3.927	14.590	20.564	1.00 51.74
MOTA	254	CG	GLN	1491	3.439	14.796	21.994	1.00 64.00
MOTA	255	CD	GLN	1491	2.545	16.039	22.180	1.00 71.35
MOTA	256	OE1	GLN	1491	2.534	16.922	21.352	1.00 77.94
MOTA	257	NE2	GLN	1491	1.824	16.083	23.289	1.00 76.51
ATOM _	.260	. C	GLN	1491	4.207	12.083	20.505	1.00 45.94
ATOM	261	0	GLN	1491	. 3.151.	11.869	19.919	1.00 48.02
MOTA	262	N	VAL	1492	4.848	11.129	21.184	1.00 41.00
MOTA	264	CA	VAL	1492	4.293	9.810	21.421	1.00 37.44
MOTA	265	CB	VAL	1492	5.235	8.665	21.025	1.00 34.74
MOTA	266	CG1	VAL	1492	4.593	7.325	21.285	1.00 28.97
MOTA	267	CG2	VAL	1492	5.632	8.769	19.553	1.00 35.78
ATOM	268	C	VAL	1492	4.014	9.621	22.901	1.00 38.67
ATOM	269	0	VAL	1492	4.907	9.769	23.735	1.00 38.62
ATOM	270	N	VAL	1493	2.776	9.276	23.250	1.00 39.98
ATOM	272	CA	VAL	1493	2.423	9.062	24.653	1.00 37.79
MOTA	273	CB	VAL	1493	1.257	9.970	25.093	1.00 37.36
ATOM	274	CG1	VAL	1493	1.489	11.403	24.689	1.00 39.11
MOTA	275	CG2	VAL	1493	-0.074	9.480	24.555	1.00 38.99
MOTA	276	С	VAL	1493	2.052	7.603	24.877	1.00 36.38
ATOM	277	0	VAL	1493	1.759	6.874	23.945	1.00 37.73
MOTA	278	N	LEU	1494	2.094	7.176	26.123	1.00 35.42
MOTA	280	CA	LEU	1494	1.718	5.817	26.483	1.00 33.65
MOTA	281	CB	LEU	1494	2.536	5.291	27.670	1.00 29.88
ATOM	282	CG	LEU	1494	2.117	3.945	28.279	1.00 30.31
MOTA	283		LEU	1494	2.103	2.844	27.244	1.00 30.83
MOTA	284	CD2	LEU	1494	3.049	3.574	29.400	1.00 32.12
ATOM	285	С	LEU	1494	0.260	5.934	26.870	1.00 34.27
ATOM	286	0	LEU	1494	-0.168	6.994	27.348	1.00 34.85
ATOM	287	N	ALA	1495	-0.527	4.898	26.608	1.00 32.20
ATOM	289	CA	ALA	1495	-1.930	4.954	26.980	1.00 29.71
ATOM	290	CB	ALA	1495	-2.724	5.722	25.930	1.00 25.48
ATOM	291	C	ALA	1495	-2.499	3.567	27.183	1.00 28.85
ATOM	292	0	ALA	1495	-1.826	2.563	26.998	1.00 27.28
ATOM	293	N	GLU	1496	-3.743	3.519	27.615	1.00 32.20
ATOM	295	CA	GLU	1496	-4.413	2.250	27.824	1.00 33.34
ATOM	296	CB	GLU	1496	-4.735	2.063	29.301	1.00 35.65
ATOM	297	CG	GLU	1496	-3.521	1.962	30.198	1.00 39.14
ATOM	298	CD	GLU	1496	-3.899	2.045	31.663	1.00 42.57
ATOM	299	OE1		1496	-4.469	3.083	32.061	1.00 42.59
ATOM	300	OE2		1496	-3.646	1.069	32.407	1.00 42.76
ATOM	301	C	GLU	1496	-5.692	2.274	26.994	1.00 33.40
ATOM	302	0	GLU	1496	-6.439	3.261	27.017	1.00 34.36
ATOM	303	N	ALA	1497	-5.875	1.247	26.177	1.00 31.67
ATOM	305	CA	ALA	1497	-7.051	1.168	25.351	1.00 31.23

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ATOM	306	CB	ALA	1497	-6.671	0.750	23.953	1.00 28.13
ATOM	307	С	ALA	1497	-8.000	0.168	25.974	1.00 32.02
ATOM	308	0	ALA	1497	-7.599	-0.954	26.261	1.00 33.45
ATOM	309	N	ILE	1498	-9.218	0.602	26.282	1.00 34.15
MOTA	311	CA	ILE	1498	-10.222	-0.294	26.854	1.00 35.89
MOTA	312	CB	ILE	1498	-11.294	0.453	27.679	1.00 35.30
ATOM	313	CG2	ILE	1498	-12.267	-0.551	28.300	1.00 32.95
ATOM	314	CG1	ILE	1498	-10.663	1.316	28.770	1.00 35.29
ATOM	315	CD1	ILE	1498	-11.656	2.262	29.419	1.00 31.69
ATOM	316	С	ILE	1498	-10.953	-0.929	25.680	1.00 38.79
ATOM	317	0	ILE	1498	-11.571	-0.227	24.877	1.00 37.46
ATOM	318	N	GLY	1499	-10.859	-2.245	25.559	1.00 43.14
ATOM	320	CA	GLY	1499	11.544	-2.918	24.477	1.00 46.90
ATOM	321	С	GLY	1499	-10.673	-3.299	23.298	1.00 49.69
ATOM	322	0	GLY	1499	-9.921	-4.269	23.387	1.00 51.47
ATOM	323	N	LEU	1500	-10.739	-2508	22.223	1.00 49.92
MOTA	325	CA	LEU	1500	-10.003	-2.765	20.973	1.00 49.62
ATOM	326	CB	LEU	1500	-8.478	-2.898	21.185	1.00 49.96
ATOM	327	CG	LEU	1500	-7.504	-1.703	21.167	1.00 49.26
ATOM	328	CD1	LEU	1500	-6.069	-2.217	21.284	1.00 47.17
MOTA	329	CD2	LEU	1500	-7.638	-0.883	19.899	1.00 47.80
ATOM	330	С	LEU	1500	-10.535	~4.027	20.275	1.00 49.49
ATOM	331	0	LEU	1500	-10.480	-5.145	20.806	1.00 47.99
ATOM	332	N	PRO	1505	-13.253	-5.837	25.284	1.00 50.58
MOTA	333	CD	PRO	1505	-13.877	-7.173	25.239	1.00 51.43
MOTA	334	CA	PRO	1505	-14.197	-4.825	25.779	1.00 48.68
MOTA	335	CB	PRO	1505	-15.548	-5.521	25.627	1.00 48.59
ATOM	336	CG	PRO	1505	-15.216	-6.944	25.940	1.00 51.66
MOTA	337	C	PRO	1505	-13.904	-4.396	27.227	1.00 44.58
MOTA	338	0	PRO	1505	-13.883	-3 202	27.531	1.00 42.73
MOTA	339	N	ASN	1506	-13.640	-5.363	28.102	1.00 42.10
MOTA	341	CA	ASN	1506	-13.337	-5.053	29.497	1.00 45.05
MOTA	342	CB	ASN	1506	-14.202	-5.893	30.434	1.00 47.04
ATOM	343	CG	ASN	1506	-15.657	-5.493	30.395	1.00 48.72
ATOM	344	OD1	asn	1506	-15.999	-4.309	30.487	1.00 50.48
MOTA	345	ND2	ASN	1506	-16.529	-6.478	30.260	1.00 51.15
MOTA	348	С	ASN	1506	-11.863	-5.251	29.836	1.00 46.50
ATOM	349	0	ASN	1506	-11.487	-5.343	31.008	1.00 46.50
ATOM	350	N	ARG	1507	-11.029	-5.284	28.806	1.00 46.99
MOTA	352	CA	ARG	1507	-9.594	-5.466	28.976	1.00 47.52
MOTA	353	CB	ARG	1507	-9.111	-6.650	28.142	1.00 54.20
MOTA	354	CG	ARG	1507	-9.327	-7.993	28.781	1.00 64.52
MOTA	355	CD	ARG	1507	-8.402	-8.180	29.963	1.00 71.17
MOTA	356	NE	ARG	1507	-8.592	-9.494	30.556	1.00 76.52
MOTA	358	CZ	ARG	1507	-8.030	-9.898	31.689	1.00 81.64
MOTA	359	NH1	ARG	1507	-7.219	-9.096	32.375	1.00 83.30
MOTA	362	NH2	ARG	1507	-8.340	-11.093	32.174	1.00 84.44
MOTA	365	C	ARG	1507	-8.871	-4.234	28.485	1.00 43.46
MOTA	366	0	ARG	1507	-9.227	-3.695	27.440	1.00 42.73
MOTA	367	N	VAL	1508	-7.912	-3.749	29.265	1.00 40.84
ATOM	369	CA	VAL	1508	-7.143	-2.598	28.830	1.00 38.27
MOTA	370	CB	VAL	1508	-6.786	-1.604	29.961	1.00 34.90

MOTA	371	CG1	VAL	1508	-8.038	-1.124	30.646	1.00 41.81
ATOM	372	CG2	VAL	1508	-5.850	-2.226	30.944	1.00 35.B9
ATOM	373	С	VAL	1508	-5.874	-3.147	28.211	1.00 36.81
ATOM	374	0	VAL	1508	-5.371	-4.191	28.637	1.00 35.13
MOTA	375	N	THR	1509	-5.393	-2.465	27.180	1.00 36.04
MOTA	377	CA	THR	1509	-4.184	-2.854	26.485	1.00 33.31
ATOM	378	CB	THR	1509	-4.503	-3.254	25.025	1.00 33.79
ATOM	379	OG1	THR	1509	-5.511	-4.275	25.014	1.00 33.98
ATOM	381	CG2	THR	1509	-3.259	-3.774	24.321	1.00 32.78
ATOM	382	С	THR	1509	-3.268	-1.627	26.453	1.00 32.37
ATOM	383	0	THR	1509	-3.718	-0.533	26.113	1.00 31.97
ATOM	384	N	LYS	1510	-2.015	-1.786	26.884	1.00 32.96
MOTA	386	CA	LYS	1510	-1.071	-0.673	26.828	1.00 33.25
MOTA	387	CB	LYS	1510	0.157	-0.902	27.699	1.00 34.65
MOTA	388	CG	LYS	1510	-0.093	-0.909	29.197	1.00 39.64
ATOM	389	CD	LYS	1510	1.237	-1.105	29.913	1.00 43.51
MOTA	390	CE	LYS	1510	1.110	-1.949	31.173	1.00 48.42
ATOM	391	NZ	LYS	1510	0.399	-1.256	32.287	1.00 53.03
ATOM	395	С	LYS	1510	-0.646	-0.550	25.370	1.00 32.26
ATOM	396	0	LYS	1510	-0.240	-1.533.	24.736	1.00 30.20
ATOM	397	N	VAL	1511	-0.760	0.665	24.849	1.00 32.28
ATOM	399	CA	VAL	1511	.0.436	0.980	23.472	1.00 30.73
MOTA	400	CB	VAL	1511	-1.738	1.140	22.666	1.00 32.25
ATOM	401	CG1	VAL	1511	-2.566	0.147	22.723	1.00 29.00
ATOM	402	CG2	VAL	1511	-2.549	2.347	23.193	1.00 29.17
MOTA	403	С	VAL	1511	0.329	2.307	23.423	1.00 30.91
ATOM	404	0	VAL	1511	0.445	3.008	24.433	1.00 31.94
ATOM	405	N	ALA	1512	0.842	2.658	22.250	1.00 27.30
ATOM	407	CA	ALA	1512	1.550	3.914	22.094	1.00 24.22
MOTA	408	CB	ALA	1512	2.921	3.694	21.493	1.00 23.39
MOTA	409	C	ALA	1512	0.698	4.769	21.181	1.00 23.62
MOTA	410	0	ALA	1512	0.116	4.271	20.228	1.00 22.69
ATOM	411	N	VAL	1513	0.605	6.054	21.484	1.00 27.51
ATOM	413	CA	VAL	1513	-0.192	6.984	20.688	1.00 30.03
MOTA	414	CB	VAL	1513	-1.359	7.613	21.522	1.00 28.31
MOTA	415	CG1	VAL	1513	-2.218	8.522	20.650	1.00 28.93
ATOM	416	CG2	VAL	1513	-2.214	6.542	22.159	1.00 26.00
ATOM	417	С	VAL	1513	0.674	8.108	20.107	1.00 31.21
ATOM	418	0	VAL	1513	1.370	8.816	20.834	1.00 29.73
ATOM	419	N	LYS	1514	0.631	8.225	18.784	1.00 33.99
ATOM.	421	CA	LYS	1514	1.342	9.258	18.037	1.00 35.44
ATOM	422	CB	LYS	1514	1.831	8.692	16.707	1.00 34.55
ATOM	423	CG	LYS	1514	2.835	7.586	16.872	1.00 35.38
ATOM	424	CD	LYS	1514	3.025	6.807	15.599	1.00 36.87
ATOM	425	CE	LYS	1514	3.457	7.710	14.438	1.00 45.19
ATOM	426	NZ	LYS	1514	4.598	8.622	14.755	1.00 44.31
MOTA	430	C	LYS	1514	0.304	10.345	17.761	1.00 35.97
MOTA	431	0	LYS	1514	-0.806	10.037	17.299	1.00 34.39
MOTA	432	N	MET	1515	0.673	11.596	18.028	1.00 38.17
MOTA	434	CA	MET	1515	-0.207	12.747	17.835	1.00 41.17
MOTA	435	CB	MET	1515	-0.901	13.098	19.145	1.00 39.54
ATOM	436	CG	MET	1515	0.075	13.428	20.255	1.00 39.11

ATOM	437	SD	MET	1515	-0.766	13.612	21.799	1.00 43.8	5
MOTA	438	CE	MET	1515	-1.212	11.937	22.087	1.00 46.1	
MOTA	439	С	MET	1515	0.612	13.939	17.391	1.00 43.6	
ATOM	440	0	MET	1515	1.834	13.905	17.445	1.00 45.7	
MOTA	441	N	LEU	1516	-0.053	14.962	16.872	1.00 48.7	
ATOM	443	CA	LEU	1516	9.640	16.175	16.448	1.00 52.2	
MOTA	444	CB	LEU	1516	-0.152	16.917	15.374	1.00 49.7	
ATOM	445	CG	LEU	1516	-0.413	16.254	14 036	1.30 48.04	
MOTA	446	CD1	LEU	1516	-1.418	17.104	13.285	1.00 48.16	
ATOM	447	CD2	LEU	1516	0.884	16.102	13.265	1.00 42.80	
MOTA	448	С	LEU	1516	0.810	17.119	17.631	1.00 55.67	
ATOM	449	0	LEU	1516	0.217	16.927	18.703	1.00 53.99	
ATOM	450	N	LYS	1517	1.580	18.174	17.402	1.00 60.97	
MOTA	452	CA	LYS	1517	1.823	19.193	18.416	1.00 65.19	
ATOM	453	CB	LYS	1517	3.274	19.668	18.344	1.00 69.34	
ATOM	454	CG	LYS	1517	4.294	18.559	18.529	1.00 72.86	
ATOM	455	CD	LYS	1517	5.646	18.935	17.929	1.00 74.91	
MOTA	456	CE	LYS	1517	6.686	17.851	18.197	1.00 74.38	
ATOM	457	NZ	LYS	1517	8.010	18.241	17.649	1.00 75.45	
ATOM	461	C	LYS	1517	0.879	20.357	18.139	1.00 65.97	
MOTA	462	0	LYS	1517	0.303	20.451	L7.053	1.00 64.59	
MOTA	463	N	SER	1518	0.776	21.270	19.098	1.00 68.20	
ATOM	465	CA	SER	1518	-0.107	22.422	18.972	1.00 71.92	:
ATOM	466	CB	SER	1518	-0.002	23.322	20.202	1.00 69.89	t
ATOM	467	C	SER	1518	0.144	23.247	17.718	1.00 74.68	
MOTA	468	O	SER	1518	-0.798	23.604	17.006	1.00 77.44	
ATOM	469	N	ASP	1519	1.417	23.493	17.422	1.00 76.04	
ATOM	471	CA	ASP	1519	1.799	24.299	16.264	1.00 76.48	
MOTA	472	CB	ASP	1519	3.126	25.011	16.539	1.00 77.59	
ATOM	473	С	ASP	1.519	1.912	23.525	14.958	1.00 75.88	
ATOM	474	0	ASP	1519	2.374	24.075	13.959	1.00 77.52	
MOTA	475	N	ALA	1520	1.486	22.265	14.956	1.00 74.39	
ATOM	477	CA	ALA	1520	1.574	21.439	13.758	1.00 72.83	
ATOM	478	CB	ALA	1520	0.930	20.079	14.010	1.00 73.06	
ATOM ATOM	479	C	ALA	1520	0.889	22.153	12.598	1.00 71.47	
ATOM	480	0	ALA	1520	-0.096	22.858	12.797	1.00 73.48	
ATOM	481	N	THR	1521	1.440	22.015	11.401	1.00 69.15	
ATOM	483	CA	THR	1521	0.858	22.653	10.234	1.00 70.05	
ATOM	484	CB	THR	1521	1.950	23.110	9.272	1.00 70.21	
ATOM	485	_	THR	1521	2.505	21.969	8.607	1.00 72.71	
ATOM	487 488	CG2 C	THR	1521	3.053	23.815	10.043	1.00 71.01	
ATOM	489	0	THR THR	1521	-0.015	21.616	9.550	1.00 70.64	
ATOM	490	N		1521	0.015	20.443	9.932	1.00 72.38	
ATOM	492		GLU	1522	-0.782	22.026	8.542	1.00 69.70	
ATOM	493	CA CB	GLU GLU	1522	-1.623	21.081	7.815	1.00 67.41	
ATOM	494	СВ	GLU	1522	-2.478	21.800	6.761	1.00 70.01	
ATOM	495	0		1522	-0.718	20.024	7.168	1.00 64.50	
ATOM ATOM	495		GLU	1522	-1.125	18.878	7.006	1.00 63.76	
ATOM	498	N CA	LYS LYS	1523	0.512	20.419	6.827	1.00 60.75	
ATOM ATOM	498	CB		1523	1.483	19.502	6.240	1.00 58.57	
ATOM ATOM	500	CB	LYS	1523	2.782	20.230	5.883	1.00 60.63	
	200	CG	LYS	1523	3.909	19.318	5.361	1.00 62.47	

	MOTA	501	CD	LYS	1523	3.459	18.461	4.168	1.00 63.35
	ATOM	502	CE	LYS	1523	4.633	17.700	3.559	1.00 66.57
	MOTA	503	NZ	LYS	1523	4.210	16.733	2.498	1.00 69.56
	MOTA	507	C	LYS	1523	. 1.763	18.441	7.281	1.00 55.98
	ATOM	508	0	LYS	1523	1.790	17.251	6.972	1.00 56.37
	MOTA	509	N	ASP	1524	1.960	18.885	8.517	1.00 52.16
	ATOM	511	CA	ASP	1524	2.211	17.980	9.630	1.00 48.91
	ATOM	512	CB	ASP	1524	2.487	18.762	10.915	1.00 50.87
	MOTA	513	CG	ASP	1524	3.865	19.401	10.928	1.00 53.00
	ATOM	514	OD1	ASP	1524	4.004	20.511	11.499	1.00 53.77
	MOTA	515	OD2	ASP	1524	4.816	18.785	10.394	1.00 56.30
	ATOM	516	C	ASP	1524	1.032	17.031	9.831	1.00 45.34
	ATOM	517	0	ASP	1524	1.221	15.858	10.176	1.00 45.63
	ATOM	518	N	LEU	1525	-0.176	17.530	9.593	1.00 40.15
	ATOM	520	CA	LEU	1525	-1.368	16.715	9.711	1.00 39.38
	MOTA	521	CB	LEU	1525	-2.624	17.588	9.633	1.00 41.66
	MOTA	522	CG	LFU	1525	-4.020	16.937	9.585	1.00 42.75
	ATOM	5 23	CD1	LEU	1525	~4.245	15.945	10.727	1.00 42.97
	MOTA	524	CD2	LEU	1525	-5.058	18 026	9.644	1.00 42.24
	MOTA	525	С	LEU	1525	-1.340	15.599	8.575	1.00 39.77
	MOTA	526	O	LEU	1525	-1.509	14.506	8.813	1.00 39.11
	ATOM	527	N	SER	1526	-1.062	16.172	7.361	1.60 39.64
	ATOM	529	CA	SER	1526	~0.998	15.320	6.181	1.00 40.65
	ATOM	530	CB	SER	1526	-0.541	16.105	4.947	1.00 43.32
	ATOM	531	OG	SER	1526	-1.398	17.190	4.656	1.00 52.41
	ATOM	533	C.	SER	1526	-0.015	14.201	6.383	1.00 39.12
	ATOM	534	0	SER	1526	-0.346	13.038	6.198	1.00 41,75
	ATOM	535	N	ASP	1527	1.203	14.553	ä.769	1.00 38.30
	ATOM	537	CA	ASP	1527	2 244	13.552	6.969	1.00 39.28
	MOTA	538	CB	ASP	1527	3.531	14.208	7.47:	1.00 41.16
	ATOM	539	CG	ASP	1527 ·	4.218	15.069	6.404	1.00 45.20
	MOTA	540	ODl	ASP	1527	3.861	14.972	5.198	1.00 43.25
	ATOM	541	OD2	ASP	1527	5.132	15.840	6.788	1.00 45.93
	ATOM	542	C	ASP	1527	1.788	12.443	7.903	1.00 37.34
	MOTA	543	0	ASP	1527	1.867	11.259	7.557	1.00 37.24
	ATOM	544	N	LEU	1528	1.224	12.535	9.036	1.00 35.88
	MOTA	546	CA	LEU	1528	0.728	11.874	10.009	1.00 35.07
	ATOM	547	CB	LEU	1528	0.185	12.606	11.242	1.00 34.38
	ATOM	548	CG	LEU	1528	-0.146	11.789	12.491	1.00 35.86
	ATOM	549	CD1	LEU	1528	1.009	10.845	12.820	1.00 34.83
	ATOM	550	CD2	LEU	1528	-0.435	12.711	13.642	1.00 29.98
	ATOM	551	С	LEU	1528	-0.351	10.977	9.374	1.00 33.31
	MOTA	552	0	LEU	1528	-0.342	9.756	9.552	1.00 34.55
	MOTA	553	N	ILE	1529	-1.236	11.575	8.585	1.00 32.16
	ATOM	555	CA	ILE	1529	-2.306	10.829	7.924	1.00 30.94
	ATOM	556	CB	ILE	1529	-3.304	11.757	7.178	1.00 27.07
	MOTA	557	CG2	ILE	1529	-4.388	10.926	6.521	1.00 26.06
	A'TOM	558	CG1	ILE	1529	-3.953	12.723	8.169	1.00 23.67
i	MOTA	559	CD1	ILE	1529	-4.877	13.736	7.526	1.00 22.34
į	ATOM	560	С	ILE	1529	-1.684	9.856	6.947	1.00 31.34
i	MOTA	561	0	ILE	1529	-2.058	8.683	6.912	1.00 33.57
i	MOTA	562	N	SER	1530	-0.703	10.331	6.191	1.00 30.74

ATOM	564	CA	SER	1530	0.007	9.496	5.230	1.00 32.04	
ATOM	565	CB	SER	1530	1.109	10.302	4.548	1.00 35.20	-
MOTA	566	OG	SER	1530	0.596	11.501	4.002	1.00 41.97	
ATOM	568	C	SER	1530	0.620	8.262	5.895	1.00 29.06	
ATOM	569	0	SER	1530	0.478	7.140	5.377	1.00 26.64	•
ATOM	570	N	GLU	1531	1.287	8.464	7.034	1.00 23.86	-
ATOM	572	CA	GLU	1531	1.918	7.367	7.759	1.00 23.86	
ATOM	573	CB	GLU	1531	2.729	7.893	8.944	1.00 25.69	
ATOM	574	CG	GLU	1531	3.501	6.803	9.701	1.00 23.65	
MOTA	575	CD	GLU	1531	4.341	7.319	10.868	1.00 26.03	-
ATOM	576	OE1	GLU	1531	4.927	6.473	11.572	1.00 25.92	
ATOM	577		GLU	1531	4.435	8.549	11.094	1.00 26.55	
MOTA	578	C	GLU	1531	0.906	6.325	8.222	1.00 25.44	 • •••
ATOM	579	0	GLU	1531	1.200	5.126	8.228	1.00 23.67	
MOTA	580	N	MET	1532	-0.285	6.788	8.600	1.00 26.39	
MOTA	582	CA	MET	1532	-1.365	5.898	9.048	1.00 26.57	
ATOM	583	CB	MET	1532	-2.473	6.720	9.714	1.00 24.81	
ATOM	584	CG	MET	1532	-3.645	5.889	10.191	1.00 27.47	
ATOM	585	SD	MET	1532	-4.969	. 5.89 9	10.860	1.00 28.43	
ATOM	586	CE	MET	1532	-5.178	8.102	9.576	1.00 24.45	
ATOM	587	С	MET	1532	-1.923	5.076	7.861	1.00 28.30	
ATOM	588	0	MET	1532	-2.048	3.850	7.933	1.00 27.95	
ATOM	589	N	GLU	1533	-2.221	5.760	6.762	1.00 28.95	
ATOM	591	CA	GLU	1533	-2.732		5.565	1.00 30.32	
MOTA	592	CB	GLU	1533	-2.983	6.143	4.476	1.00 25.40	
ATOM	593	CG	GLU	1533	-4.064	7.127	4.852	1.00 26.09	
ATOM	594	CD	GLU	1533	-5.402	6.461	5.119	1.00 25.89	
ATOM	595		GLU	1533	-5.913	5.745	4.240	1.00 27.24	
ATOM	596		GLU	1533	-5.964	6.6€2	6.209	1.00 30.00	
ATOM	597	C	GLU	1533	-1.723	4.089	5.093	1.00 31.64	
ATOM	598	0	GLU	1533	-2.080	2.983	4.706	1.00 33.57	
ATOM	599	N	MET	1534	-0.455	4.472	5.166	1.00 33.57	
ATOM	601	CA	MET	1534	0.664	3.618	4.793	1.00 32.86	
ATOM	602	CB	MET	1534	1.957	4.390	5.003	1.00 32.89	
MOTA	603	CG	MET	1534	3.159	3.559	4.851	1.00 39.27	
ATOM	604	SD	MET	1534	3.577	3.513	3.164	1.00 51.24	
ATOM ATOM	605 606	CE	MET MET	1534 1534	5.153	4.319	3.204	1.00 44.97	
ATOM	607	0	MET	1534	0.670	2.373	5.681 5.198	1.00 31.84 1.00 33.78	
ATOM	608	N	MET	1535	0.816 0.509	1.250 2.571	6.982	1.00 33.78	
MOTA	610	CA	MET	1535	0.469	1.453	7.902		
ATOM	611	CB	MET	1535	0.419	1.455	9.352	1.00 28.83	
ATOM	612	CG	MET	1535	1.717	2.540	9.850	1.00 21.79	
ATOM	613	SD	MET	1535	1.722	2.764	11.628	1.00 21.30	
ATOM	614	CE	MET	1535	1.681	4.534	11.727	1.00 22.97	
ATOM	615	C	MET	1535	-0.725	0.540	7.572	1.00 23.90	
ATOM	616	0	MET	1535	-0.723	-0.694	7.706	1.00 30.33	
ATOM	617	N	LYS	1536	-1.823	1.135	7.104	1.00 33.31	•
MOTA	619	CA	LYS	1536	-3.011	0.364	6.732	1.00 28.91	*
ATOM	620	CB	LYS	1536	-4.176	1.289	6.413	1.00 25.52	
ATOM	621	CG	LYS	1536	-4.689	2.080	7.579	1.00 25.52	_
ATOM	622	CD	LYS	1536	-5.810	2.979	7.127	1.00 21.46	
ALON	UZZ	CD	пто	1330	-2.610	2.3/3	1.121	1.00 13.89	

MOTA 623 CE LYS 1536 -6.414 3.717 8.288 1.00 23.50 ATOM NZ LYS 624 1536 -7.469 4.668 7.850 1.00 23.53 MOTA 628 C LYS 1536 -2.765 -0.542 5.530 1.00 29.09 **ATOM** 629 0 LYS 1536 -1.708 -3.127 5.550 1.00 34.02 **ATOM** 630 N MET 1537 -0.009 -2.141 4.488 1.00 29.03 MOTA CA MET 1537 -0.792 632 -1.869 3.288 1.00 30.13 **ATOM** 633 CB MET 1537 -1.315 0.111 2.177 1.00 31.96 **ATOM** 634 CG MET 1537 -2.304 1.114 1.589 1.00 35.15 ATOM 635 SD MET 1537 -3.757 0.380 0.787 1.00 41.18 -3.026 **ATOM** 636 CE MET 1537 -0.360 -0.666 1.00 43.05 **ATOM** 1537 637 C MET -0.905 -1.946 3.531 1.00 30.22 **ATOM** 638 0 MET 1537 -1.118 -3.051 3.045 1.00 30.88 **ATOM** 639 N ILE 1538 0.164 -1.686 4.275 1.00 30.91 ATOM 641 CA ILE 1538 1.192 -2.701 4.536 1.00 30.29 **ATOM** 642 CB ILE 1538 2.429 -2.082. 5.221 1.00 28.64 ATOM 643 CG2 ILE 1538 3.493 -3.142 1.00 29.84 5.453 ATOM 644 ILE CG1 1538 3.025 -1.030 4.287 1.00 32.82 ATOM ILE 645 CD1 1538 4.358 -0.446 4.763 1.00 38.38 ATOM 646 C ILE 1538 0.759 -4.000 5.237 1.00 29.07 **ATOM** 647 ILE 0 1538 1.229 -5.078 4.876 1.00 28.30 ATOM 648 N GLY 1539 -0.178 -3.925 6.174 1.00 27.61 **ATOM** 650 CA GLY 1539 -0.592 -5.147 6.849 1.00 26.22 ATOM 651 С GLY 1539 0.273 -5.484 8.055 1.00 25.67 **ATOM** 652 0 GLY 1539 -4.906 1.345 8.241 1.00 28.05 MOTA 653 LYS 1540 N -0.150 -6.493 8.819 1.00 23.80 MOTA 655 CA LYS 1540 0.532 -6.876 10.046 1.00 21.77 **ATOM** CB LYS 1540 656 -0.491 -7.436 11.045 1.00 20.04 **ATOM** 657 CG LYS 1540 -1.505 -6.435 11.480 1.00 24.45 **ATOM** 658 CD LYS 1540 -2.472 : -6.997 12.488 1.00 32.57 **ATOM** 659 CE LYS 1540 -3.516 -5.946 12.882 1.00 35.05 **ATOM** 660 ΝZ LYS 1540 -2.959 -4.850 13.733 1.00 39.81 **ATOM** 664 C LYS 1540 1.669 -7.862 9.958 1.00 20.19 **ATOM** 665 0 LYS 1540 1.671 -8.738 9.099 1.00 21.80 MOTA HIS 666 N 1541 2.626 -7.722 10.876 1.00 19.98 ATOM 668 CA HIS 1541 3.770 -8.626 11.000 1.00 22.43 MOTA CB HIS 669 1541 4.854 -8.374 9.965 1.00 22.34 MOTA 670 CG HIS 1541 5.892 -9.455 9.923 1.00 20.68 MOTA CD2 HIS 671 1541 5.906 -10.654 9.295 1.00 20.60 MOTA 672 ND1 HIS 1541 7.074 -9.382 10.633 1.00 23.67 MOTA 7.771 -10.490 674 CE1 HIS 1541 10.444 1.00 23.35 MOTA 675 NE2 HIS 1541 7.087 -11.278 9.634 1.00 22.04 ATOM 677 C HIS 1541 4.385 -8.477 12.376 1.00 27.21 **ATOM** 678 0 HIS 1541 4.538 -7.367 12.885 1.00 31.33 **ATOM** 679 N LYS 1542 4.726 -9.619 12.958 1.00 29.25 MOTA 681 CA LYS 1542 5.319 -9.698 14.285 1.00 30.39 MOTA 682 LYS CB 1542 5.660 -11.151 14.610 1.00 33.76 **ATOM** 683 CG LYS 1542 6.232 -11.370 15.994 1.00 42.16 **ATOM** 684 CD LYS 1542 6.400 -12.833 16.230 1.00 49.69 MOTA 685 CE LYS 1542 7.040 -13.499 14.988 1.00 57.71 ATOM 686 NZ LYS 1542 7.499 -14.904 15.237 1.00 62.05 MOTA 690 С LYS 1542 6.515 -8.808 14.462 1.00 27.21 ATOM 691 0 LYS 1542 6.690 -8.232 15.522 1.00 29.68

ATOM	692	N	ASN	1543	7.293	-8.619	13.410	1.00 23.81
ATOM	694	CA	asn	1543	8.472	-7.787	13.537	1.00 24.70
MOTA	695	CB	ASN	1543	9.697	-8.550	13.031	1.00 24.68
ATOM	696	CG	ASN	1543	9.914	-9.855	13.793	1.00 24.82
MOTA	697		ASN	1543	9.734	-10.942	13.239	1.00 27.33
ATOM	698	ND2	ASN	1543	10.255	-9.758	15.078	1.00 16.75
ATOM	701	С	ASN	1543	8.444	-6.326	13.032	1.00 24.93
MOTA	702	0	ASN	1543	9.469	-5.781	12.623	1.00 26.76
ATOM	703	N	ILE	1544	7.276	-5.692	13.088	1.00 24.21
ATOM	705	CA	ILE	1544	7.121	-4.281	12.710	1.00 21.87
MOTA	706	CB	ILE	1544	6.626	-4.095	11.240	1.00 23.23
ATOM	707	CG2	ILE	1544	7.549	-4.837	10.267	1.00 23.87
ATOM	708	CG1		1544	5 182	-4.580	11.063	1.00 22.57
ATOM	709		ILE	1544	4.639	-4.342	9.659	1.00 17.59
ATOM	710	С	ILE	1544	6.122	-3.656	13.696	1.00 21.64
ATOM	711	0	ILE	1544	5.399	-4.377	14.397	1.00 21.00
ATOM	712	N	ILE	1545	6.167	-2.340	13.856	1.00 21.59
ATOM	714	CA	ILE	1545	5.214	-1.687	14.746	1.00 24.05
ATOM	715	СВ	ILE	1545	5.641	-0.242	15.138	1.00 23.68
ATOM	716	CG2	ILE	1545	4.473	0.500	15.831	1.00 21.90
ATOM	717	CG1		1545	ნ. 880	-0.284	16.050	1.00 21.94
ATOM	718	CD1		1545	6.643	-0.808	17.446	1.00 9.18
ATOM	719	C	ILE	1545	3.914	-1.641	13.955	1.00 25.08
MOTA	720	0	ILE	1545	3.842	-1.001	12.897	1 00 26.68
ATOM	721	N	ASN	1546	2.909	-2.358	14.455	1.00 25.88
ATOM	723	CA	ASN	1546	1.602	-2.424	13.800	1.00 24.61
ATOM	724	CB	ASN	1546	0.944	-3.793	14.005	1 00 23.18
ATOM	725	CG	ASN	1546	1.759	-4.923	13.434	1.00 21.54
ATOM	726	OD1		1546	1.884	-5.059	12.214	1.00 21.52
ATOM ATOM	725	ND2		1546	2.319	-5.748	14.313	1.00 18.83
ATOM	730	C	ASN	1546	0.646	-1.368	14.292	1.00 23.02
MOTA	731 732	O N	ASN LEU	1546	0.739	-0.911	15.429	1.00 25.66
ATOM	734	CA	LEU	1547	-0.285	-1.014	13.422	1.00 24.45
ATOM	735	CB	LEU	1547 1547	-1.336 -1.819	-0.041	13.692 12.360	1.00 24.27
ATOM	736	CG	LEU	1547	-3.012	0.553		1.00 18.04
ATOM	737	CD1		1547	-2.630	1.515 2.928	12.343 12.842	1.00 19.96
ATOM	738	CD2		1547	-3.555	1.570	10.924	1.00 10.60 1.00 16.44
ATOM	739	C	LEU	1547	-2.469	-0.826	14.384	1.00 26.95
ATOM	740	0	LEU	1547	-2.835	-1.934	13.956	1.00 27.38
ATOM	741	N	LEU	1548	-2.998	-0.260	15.460	1.00 26.61
ATOM	743	CA	LEU	1548	-4.063	-0.902	16.222	1.00 26.25
ATOM	744	СВ	LEU	1548	-3.717	-0.951	17.721	1.00 22.48
ATOM	745	CG	LEU	1548	-2.370	-1.553	18.117	1.00 20.24
ATOM	746	CD1		1548	-2.282	-1.656	19.616	1.00 19.27
ATOM	747	CD2		1548	-2.175	-2.929	17.492	1.00 19.27
ATOM	748	C	LEU	1548	-5.401	-0.198	16.017	1.00 26.75
ATOM	749	0	LEU	1548	-6.447	-0.837	16.036	1.00 25.56
ATOM	750	N	GLY	1549	-5.367	1.115	15.823	1.00 25.78
ATOM	752	CA	GLY	1549	-6.607	1.843	15.616	1.00 25.80
ATOM	753	C.	GLY	1549	-6.319	3.324	15.490	1.00 23.30
ATOM	754	ō	GLY	1549	-5.148	3.716	15.405	1.00 28.05
		-						20.03

MOTA	755	N	ALA	1550	-7.369	4.143	15.530	1.00 27.34
MOTA	757	CA	ALA	1550	-7.212	5.582	15.414	1.00 25.85
MOTA	758	CB	ALA	1550	-6.925	5.947	13.978	1.00 23.09
MOTA	759	С	ALA	1550	-8.430	6.353	15.897	1.00 26.58
MOTA	760	0	ALA	1550	-9.562	5.866	15.797	1.00 28.26
MOTA	761	N	CYS	1551	-8.182	7.551	16.429	1.00 26.30
ATOM	763	CA	CYS	1551	-9.227	8.471	16.899	1.00 28.29
ATOM	764	CB	CYS	1551	-8.966	8.952	18.342	1.00 27.12
MOTA	765	SG	CYS	1551	-9.101	7.681	19.630	1.00 27.09
MOTA	766	C	CYS	1551	-9.092	9.646	15.934	1.00 28.57
MOTA	767	0	CYS	1551	-8.156	10.436	16.044	1.00 26.80
MOTA	768	N	THR	1552	-9.966	9.699	14.933	1.00 29.27
MOTA	770	CA	THR	1552	-9.889	10.736	13.921	1.00 29.30
MOTA	771	CB	THR	1552	- 9.779	10.110	12.495	1.00 27.19
ATOM	772	OG1	THR	1552	-10.978	9.393	12.191	1.00 26.68
MOTA	774	CG2	THR	1552	-8.629	9.133	12.414	1.00 27.00
ATOM	775	С	THR	1552	-11.045	11.716	13.905	1.00 29.86
MOTA	776	0	THR	1552	-10.918	12.838	13.403	1.00 30.69
MOTA	777	N	GLN	1553	-12.201	11.268	14.369	1.00 31 21
MOTA	779	CA	GLN	1553	-13.374	12.124	14.329	1.00 34.31
MOTA	780	CB	GLN	1553	-14.641	11.279	14.147	1.00 33.00
MOTA	781	CG	GLN	1553	-14.714	10.530	12.820	1.00 34.68
ATOM	782	CD	GLN	1553	-14.584	11.453	11.617	1.00 39.26
ATOM	783	OE1	GLN	1553	-15.300	12.449	11.506	1.00 43.55
ATOM	784	NE2	GLN	1553	-13.668	11.129	10.718	1.00 37.56
ATOM	787	С	GLN	1553	-13.502	13.040	15.526	1.00 36.86
ATOM	788	0	GLN	1553	-13.030	12.714	16.613	1.00 34.88
ATOM	789	N	ASP	1554	-14.122	14.195	15.290	1.00 40.73
ATOM	791	CA	ASP	1554	-14.369	15.202	16.3:3	1.00 42.49
MOTA	792	CB	ASP	1554	-15.693	14.913	17.028	1.00 46.26
MOTA	793	CG	ASP	1554	-16.907	15.174	16.153	1.00 51.14
MOTA	794		ASP	1554	-17.686	16.097	16.488	1.00 57.62
ATOM	795	OD2		1554	-17.092	14.463	15.146	1.00 55.72
ATOM	796	С	ASP	1554	-13.249	15.299	17.336	1.00 42.31
ATOM	797	0	ASP	1554	-13.443	14.955	18.501	1.00 43.61
MOTA	798	N	GLY	1555	-12.077	15.753	16.902	1.00 41.03
MOTA	800	CA	GLY	1555	-10.960	15.864	17.823	1.00 37.98
ATOM	801	С	GLY	1555	-9.605	15.674	17.167	1.00 38.30
ATOM	802	0	GLY	1555	-9.533	15.478	15.953	1.00 37.28
ATOM	803	N	PRO	1556	-8.511	15.693	17.961	1.00 37.62
ATOM	804	CD	PRO	1556	-8.575	15.755	19.429	1.00 37.23
ATOM	805	CA	PRO	1556	-7.123	15.533	17.500	1.00 33.79
ATOM	806	CB	PRO	1556	-6.296	15.748	18.773	1.00 33.33
ATOM	807	CG		1556	-7.254	16.353	19.770	1.00 36.99
ATOM	808	C	PRO	1556	-6.891	14.134	16.990	1.00 33.57
ATOM	809	0	PRO	1556	-7.378	13.175	17.568	1.00 32.10
ATOM	810	N	LEU	1557	-6.168	14.031	15.884	1.00 33.23
ATOM	812	CA	LEU	1557	-5.859	12.745	15.300	1.00 34.20
ATOM	813	CB	LEU	1557	-5.173	12.950	13.944	1.00 32.88
ATOM	814	CG	LEU	1557	-4.674	11.716	13.183	1.00 29.78
ATOM	815	CD1		1557	-5.810	10.730	12.943	1.00 29.22
ATOM	816	CD2	LEU	1557	-4.085	12.161	11.880	1.00 28.17

ATOM	817	С	LEU	1557	-4.950	11.927	16.225	1.00 36.29
ATOM	818	0	LEU	1557	-3.847	12.365	16.580	1.00 37.50
ATOM	819	N	TYR	1558	-5.427	10.765	16.658	1.00 35.35
ATOM	821	CA	TYR	1558	-4.619	9.890	17.495	1.00 33.09
ATOM	822	CB	TYR	1558	-5.323	9.516	18.805	1.00 34.16
ATOM	823	CG	TYR	1558	-5.363	10.629	19.806	1.00 34.40
MOTA	824	CD1	TYR	1558	-6.364	10.688	20.771	1.00 33.23
MOTA	825	CEl	TYR	1558	-6.438	11.747	21.663	1.00 34.52
MOTA	826	CD2	TYR	1558	-4.426	11.655	19.757	1.00 37.30
ATOM	827	CE2	TYR	1558	-4.488	12.715	20.640	1.00 38.44
ATOM	828	CZ	TYR	1558	-5.494	12.762	21.587	1.00 36.17
ATOM	829	OH	TYR	1558	-5.561	13.848	22.431	1.00 34.28
ATOM	831 -	C	TYR	1558	-4.379	8.627	16.700	1.00 31.12
MOTA	832	0	TYR	1558	-5.329	7.980	16.255	1.00 29.83
MOTA	833	N	VAL	1559	-3.109	8.321	16.468	1.00 29.60
MOTA	835	CA	VAL	1559	-2.727	7.115	15.753	1.00 27.08
MOTA	836	CB	VAL	1559	-1.647	7.420	14.704	1.00 24.96
MOTA	837	CG1	VAL	1559	-1281	6.149	13.926	1.00 24 36
MOTA	838	CG2	VAL	1559	-2.147	8.525	13.765	1.00 19.21
MOTA	839	С	VAL	1559	-2.238	6.102	16.794	1.00 25.65
ATOM	840	0	VAL	1559	-1.169	6.257	17.389	1.00 24.97
ATOM	841	N	ILE	1560	-3.067	5.095	17.046	1.00 25.91
ATOM	843	CA	ILE	1560	-2.777	4.062	18.042	1.00 26.94
ATOM	844	CB	ILE	1560	-4.081	3.530	18.637	1.00 24.89
ATOM	845	CG2	ILE	1560	-3.785	2.744	19.900	1.00 17.89
ATOM	846	CG1	ILE	1560	-5.028	4.707	18.907	1.00 22,84
ATOM	847	CD1	ILE	1560	-6.450	4.304	19.163	1.00 22.51
MOTA	848	C	ILE	1560	-1.955	2.896	17.467	1.00 30.61
MOTA	849	0	ILE	1560	-2.445	2.111	16.636	1.00 31.41
MOTA	850	N	VAL	1561	-0.698	2.811	17.890	1.00 30.26
MOTA	852	CA	VAL	1561	0.222	1.779	17.429	1.00 29.39
ATOM	853	CB	VAL	1561	1.466	2.437	16.730	1.00 30.18
MOTA	854	CG1	VAL	3.561	1.030	3.188	15.475	1.00 20.60
ATOM	855	CG2	VAL	1561	2.148	3.415	17.675	1.00 32.91
ATOM	856	С	VAL	1561	0.662	0.870	18.588	1.00 27.40
ATOM	857	0	VAL	1561	0.323	1.128	19.742	1.00 29.33
ATOM	858	N	GLU	1562	1.381	-0.209	18.279	1.00 24.75
MOTA	860	CA	GLU	1562	1.852	-1.142	19.308	1.00 22.64
ATOM	861	CB	GLU	1562	2.426	-2.410	18.676	1.00 17.97
ATOM	862	CG	GLU	1562	1.365	-3.282	18.029	1.00 24.33
MOTA	863	CD	GLU	1562	1.909	-4.552	17.383	1.00 26.80
MOTA	864	OE1		1562	1.247	-5.592	17.507	1.00 33.32
ATOM	865	OE2		1562	2.974	-4.538	16.722	1.00 25.62
MOTA	B66	C	GLU	1562	2.885	-0.534	20.259	1.00 25.09
MOTA	867	0	GLU	1562	3.638	0.355	19.899	1.00 23.82
MOTA	868	N	TYR	1563	2.897	-1.023	21.491	1.00 28.01
MOTA	870	CA	TYR	1563	3.805	-0.539	22.512	1.00 26.93
ATOM	871	CB	TYR	1563	3.045	-0.428	23.829	1.00 27.19
MOTA	872	CG	TYR	1563	3.868	0.008	25.009	1.00 27.72
ATOM	873	CD1	TYR	1563	4.581	1.196	24.976	1.00 30.61
MOTA	874	CE1	TYR	1563	5.303	1.620	26.069	1.00 33.05
ATOM	875	CD2	TYR	1563	3.908	-0.753	26.176	1.00 25.77

ATOM	876	CE2	TYR	1563	4.626	-0.344	27.267	1.00 26.81
ATOM	877	CZ	TYR	1563	5.329	0.845	27.210	1.00 32.81
ATOM	878	OH	TYR	1563	6.091	1.271	28.276	1.00 40.16
MOTA	880	С	TYR	1563	4.989	-1.487	22.675	1.00 28.73
ATOM	881	0	TYR	1563	4.815	-2.704	22.735	1.00 27.05
MOTA	882	N	ALA	1564	6.189	-0.908	22.743	1.00 29.89
ATOM	884	CA	ALA	1564	7.453	-1.634	22.916	1.00 28.50
MOTA	885	CB	ALA	1564	8.392	-1.349	21.721	1.00 27.54
MOTA	886	C	ALA	1564	8.036	-1.092	24.229	1.00 27.05
ATOM	887	0	ALA	1564	8.790	-0.129	24.249	1.00 31.20
MOTA	888	N	SER	1565	7.650	-1.706	25.333	1.00 27.11
MOTA	890	CA	SER	1565	8.062	-1.251	26.652	1.00 28.91
ATOM	891	CB	SER	1565	7.501	-2.152	27.729	1.00 27.33
ATOM	892	OG	SER	1565	8.108	-3.419	27.650	1.00 26.58
ATOM	894	C	SER	1565	9.530	-1.085	26.915	1.00 30.19
ATOM	895	0	SER	1565	9.897	-0.330	27.810	1.00 33.44
ATOM	896	N	LYS	1566	10.368	-1.801	26.178	1.00 30.99
ATOM	898	CA	LYS	1566	11.798	-1.708	26.410	1.00 30.50
ATOM	899	CB	LYS	1566	12.452	-3.082	26.335	1.00 30.38
ATOM	900	CG	LYS	1566	12.037	-3.943	27.507	1.00 27.83
ATOM	901	CD	LYS	1566	12.605	-5.339	27.457	1.00 32.36
ATOM	902	CE	LYS	1566	12.345	-6.024	28.784	1.00 30.57
ATOM	903	NZ	LYS	1566	12.651	-7.460	28.722	1.00 34.82
MOTA	907	С	LYS	1566	12.526	-0.678	25.573	1.00 30.39
MOTA	908	0	LYS	1566	13.755	-0.567	25.640	1.00 32.53
ATOM	909	N	GLY	1567	11.753	0.127	24.851	1.00 29.45
ATOM	911	CA	GLY	1567	12.319	1.184	24.035	1.00 29.17
ATOM	912	C	GLY	1567	13.079	0.742	22.806	1.00 28.14
MOTA	913	Ü	GLY	1567	12.875	-0.364	22.324	1.00 27.70
MOTA	914	N	ASN	1568	13.975	1.601	22.320	1.00 29.48
MOTA	916	CA	ASN	1568	14.754	1.308	21.121	1.00 30.00
ATOM	917	CB	ASN	1568	15.271	2.591	20.464	1.00 28.53
ATOM	918	CG	ASN	1568	16.342	3.285	21.281	1.00 30.13
ATOM	919	OD1	ASN	1568	17.305	2.670	21.730	1.00 31.50
ATOM	920	ND2	ASN	1568	16.212	4.591	21.420	1.00 30.91
ATOM	923	C	ASN	1568	15.892	0.333	21.352	1.00 28.83
MOTA	924	0	ASN	1568	16.371	0.201	22.472	1.00 29.87
MOTA	925	N	LEU	1569	16.346	-0.300	20.274	1.00 27.43
MOTA	927	CA	LEU	1569	17.417	-1.291	20.323	1.00 29.95
ATOM	928	CB	LEU	1569	17.511	-2.022	18.972	1.00 28.96
MOTA	929	CG	LEU	1569	18.508	-3.173	18.797	1.00 30.82
MOTA	930	CD1	LEU	1569	18.431	-4.211	19.939	1.00 28.31
ATOM	931	CD2	LEU	1569	18.244	-3.819	17.461	1.00 25.70
ATOM	932	С	LEU	1569	18.805	-0.779	20.754	1.00 29.74
ATOM	933	0	LEU	1569	19.530	-1.484	21.447	1.00 28.35
MOTA	934	N	ARG	1570	19.179	0.427	20.341	1.00 31.42
ATOM	936	CA	ARG	1570	20.485	0.985	20.703	1.00 32.81
ATOM	937	СВ	ARG	1570	20.639	2.395	20.115	1.00 31.01
ATOM	938	CG	ARG	1570	21.922	3.091	20.543	1.00 35.33
MOTA	939	CD	ARG	1570	21.918	4.581	20.212	1.00 38.30
ATOM	940	NE	ARG	1570	20.700	5.272	20.649	1.00 47.77
ATOM	942	CZ	ARG	1570	20.393	5.595	21.912	1.00 53.56
				· -		5.355	,	

ATOM	943		ARG	1570	21.212	5.304	22.931	1.00 51.30	
ATOM	946		ARG	1570	19.245	6.223	22.161	1.00 51.34	
MOTA	949	С	ARG	1570	20.620	1.034	22.230	1.00 35.61	
MOTA	950	0	ARG	1570	21.548	0.455	22.814	1.00 34.40	
MOTA	951	N	GLU	1571	19.677	1.724	22.863	1.00 36.79	
ATOM	953	CA	GLU	1571	19.637	1.855	24.311	1.00 37.35	
ATOM	954	CB	GLU	1571	18.403	2.662	24.725	1.00 41.36	
MOTA	955	CG	GLU	1571	18.407	4.118	24.267	1.00 49.97	
MOTA	956	CD	GLU	1571	17.048	4.823	24.459	1.00 59.14	
ATOM	9 57	OE1	GLU	1571	15.991	4.133	24.595	1.00 59.21	
ATOM	958	OE2	GLU	1571	17.043	6.081	24.446	1.00 59.41	
ATOM	959	С	GLU	1571	19.593	0.459	24.948	1.00 37.09	
ATOM	960	0-	GLU	::1571	20.327	0.172	25.892	1.00 37.70	
ATOM	961	N	TYR	1572	18.750	-0.405	24.400	1.00 35.08	
ATOM	963	CA	TYR	1572	18.591	-1.766	24.878	1.00 32.72	
ATOM	964	CB	TYR	1572	17.571	-2.499	23.995		
ATOM	965	CG	TYR	1572	17.376	-3.973	24.309	1.00 31.62	
ATOM	966		TYR	1572	16.392	-4.378	25.187	1.00 25.69	
ATOM	967		TYR	1572	16.180			1.00 27.87	
ATOM	968		TYR	1572	18.151	-5.711 -4.341	25.458	1.00 28.57	
ATOM	969		TYR	1572	17.948	-4.341 -6.284	23.703	1.00 22.18	
ATOM	970	cz	TYR	1572	16.954		23.969	1.00 25.06	
ATOM	971	ОН	TYR	1572	16.732	-6.659 -7.985	24.852	1.00 25.65	
ATOM	973	C	TYR	1572	19.904		25.143	1.00 25.29	
ATOM	974	ō	TYR	1572	20.186	-2.525	24.871	1.00 34.57	
ATOM	975	N	LEU	1573	20.692	-3.309 -2.338	25.796 23.812	1.00 35.05	
ATOM	977	CA	LEU	1573	21.970	-3.033		1.00 33.34	
ATOM	978	CB	LEU	1573	22.487	-3.018	23.712 22.273	1.00 33.00	
ATOM	979	CG	LEU	1573	21.833	-3.888	21.198	1.00 29.86	
ATOM	980	CD1		1573	. 22.339	-3.448	19.840	1.00 23.37	
ATOM	981	CD2		1573	22.129	-5.354		1.00 16.57	
MOTA	982	C	LEU	1573	. 22.997	-2.417	21.426 24.655	1.00 20.31	
ATOM	983	ō	LEU	1573	23.752	-3.134		1.00 36.57	
ATOM	984	N	GLN	1574	23.003	-1.090	25.311	1.00 39.00	
ATOM	986	CA	GLN	1574	23.942		24.735	1.00 37.26	
ATOM	987	CB	GLN	1574		-0.399	25.608	1.00 37.50	
ATOM	988	CG	GLN	1574	23.844 24.526	1.110 1.582	25.394	1.00 36.96	
ATOM	989	CD CG	GLN	1574			24.113	1.00 39.10	
ATOM	990	OE1		1574	24.289	3.054	23.801	1.00 40.63	
ATOM	991	NE2		1574	23.697	3.796	24.595	1.00 38.68	
ATOM	994	C	GLN	1574	24.736	3.480	22.625	1.00 38.62	
ATOM	995	0	GLN	1574	23.687 24.600	-0.759	27.073	1.00 38.27	
ATOM	996	N	ALA			-1.144	27.801	1.00 39.43	
ATOM	998		ALA	1575	22.422	-0.731	27.469	1.00 38.80	
ATOM				1575	22.021	-1.044	28.831	1.00 39.51	
	999		ALA	1575	20.551	-0.714	29.024	1.00 36.89	
ATOM	1000		ALA	1575	22.304	-2.484	29.275	1.00 40.89	
MOTA	1001		ALA	1575	22.006	-2.842	30.417	1.00 44.53	
ATOM	1002		ARG	1576	22.857	-3.317	28.395	1.00 39.11	
ATOM	1004		ARG	1576	23.148	-4.703	28.768	1.00 38.24	
ATOM	1005		ARG	1576	22.234	-5.669	28.019	1.00 38.42	
ATOM	1006		ARG	1576	20.794	-5.518	28.472	1.00 39.73	
ATOM	1007	CD	ARG	1576	19.838	-6.352	27.687	1.00 37.87	

ATOM 1008 NE ARG 1576 18.489 -6.260 28.235 1.00 41.03 ATOM 1010 ARG CZ 1576 17.830 -5.123 28.436 1.00 43.27 **ATOM** 1011 NH1 ARG 1576 18.399 -3.961 28.143 1.00 42.64 **ATOM** 1014 NH2 ARG 1576 1.00 46.13 16.573 -5.152 28.877 **ATOM** 1017 C ARG 1576 24.604 -5.076 28.612 1.00 39.77 **ATOM** 1018 0 ARG 1576 24.978 -6.256 28.623 1.00 40.25 MOTA 1019 N ARG 1577 25.428 -4.042 28.501 1.00 40.39 MOTA 1021 CA ARG 1577 26.866 -4.194 28.388 1.00 40.42 MOTA 1022 CB ARG 1577 27.485 -2.871 27.952 1.00 37.67 MOTA 1023 CG ARG 1577 27.247 -2.477 26.526 1.00 36.22 ATOM 1024 CD ARG 27.857 1577 -1.113 26.287 1.00 35.55 ATOM 1025 ·NE ARG 1577 27.971 -0.797 24.866 1.00 38.72 **ATOM** 1027 CZ ARG 1577 28.395 0.369 24.384 1.00 37.57 MOTA 1028 NH1 ARG 1577 28.754 1.352 25.205 1.00 37.49 MOTA 1031 NH2 ARG 1577 28.449 0.562 23.074 1.00 39.58 **ATOM** 1034 C ARG 1577 27.449 -4.548 29.760 1.00 42.45 ATOM 1035 0 ARG 1577 26.878 -4.180 30.801 1.00 42.57 ATOM 1036 1578 N PRO 28.564 -5.296 29.797 1.00 43.36 **ATOM** 1037 CD PRO 1578 29.270 -5.985 28.692 1.00 42.43 MOTA 1038 CA **PRO** 1578 29.159 -5.648 31.082 1.00 43.08 MOTA 1039 CB PRO 1578 30.225 -6.676 30.709 1.00 40.33 **ATOM** 1040 CG **PRO** 1578 30.600 29.331 -6.300 1.00 40.71 ATOM 1041 С PRO 1578 29.768 31.666 -4.373 1.00 42.44 ATOM 1042 0 PRO 1578 30.261 -3.525 30.922 1.00 41.24 **ATOM** 1043 N PRO 1579 29.705 -4.205 32.993 1.00 44.57 **MOTA** 1044 CD PRO 1579 29.169 -5.143 33.994 1.00 46.68 **ATOM** 1045 CA PRO 1579 30.251 -3.017 33.654 1.00 44.89 **ATOM** 1046 CB PRO 1579 30.088 -3.356 35.134 1.00 45.31 **ATOM** 1047 -4.224 CG PRO 1579 28.865 35.142 1.00 44.45 **ATOM** 1048 С PRO 1579 31.711 -2.767 33.289 1.09 45.17 **ATOM** 1049 0 PRO 1579 32.620 -3.257 33.953 1.00 47.72 **ATOM** 1050 N ALA 1592 19.075 -5.384 32.475 1.00 49.23 **ATOM** 1052 ALA CA 1592 20.500 -5.078 32.354 1.00 50.33 MOTA 1053 ALA CB 1592 20.954 -4.184 33.503 1.00 51.83 MOTA 1054 C ALA 1592 21.412 -6.308 32.251 1.00 50.65 **ATOM** 1055 0 ALA 1592 22.621 -6.166 32.044 1.00 51.55 MOTA 1056 N ALA 1593 20.849 -7.505 32.409 1.00 49.06 ATOM 1058 CA ALA 1593 21.638 -8.735 32.294 1.00 48.07 ATOM 1059 CB ALA 1593 20.773 -9.953 32.579 1.00 47.87 MOTA 1060 C ALA 1593 22.25B -8.840 30.891 1.00 47.59 ATOM 1061 0 ALA 1593 21.664 -8.426 29.894 1.00 49.09 **ATOM** 1062 N GLN 1594 23.465 -9.388 30.830 1.00 47.30 **MOTA** 1064 CA GLN 1594 24.186 -9.553 29.569 1.00 45.32 MOTA 1065 CB GLN 1594 25.576 -10.118 29.837 1.00 44.82 MOTA 1066 CG GLN 1594 26.523 -9.166 30.542 1.00 49.34 **ATOM** 1067 CD GLN 1594 27.751 -9.877 1.00 52.40 31.111 MOTA 1068 OE1 GLN 1594 28.264 -10.847 30.537 1.00 51.16 ATOM 1069 NE2 GLN 1594 28.209 -9.408 32.265 1.00 54.00 **ATOM** 1594 1072 С GLN 23.474 -10.432 28.539 1.00 45.00 ATOM 1073 0 GLN 22.780 -11.393 1594 28.876 1.00 45.28 MOTA 1074 N LEU 1595 23.684 -10.104 27.273 1.00 45.08 **ATOM** 1076 CA LEU 1595 23.084 -10.828 26.169 1.00 44.65

ATOM	1077	CB	LEU	1595	22.758	-9.864	25.023	1.00 43.08
ATOM	1078	CG	LEU	1595	21.619	-8.877	25.295	1.00 43.22
ATOM	1079		LEU	1595	21.855	-7.563	24.564	1.00 41.25
ATOM	1080	CD2	LEU	1595	20.276	-9.510	24.918	1.00 41.96
ATOM	1081	С	LEU	1595	24.044	-11.885	25.685	1.00 44.58
MOTA	1082	0	LEU	1595	25.252	-11.661	25.632	1.00 44.62
MOTA	1083	N	SER	1596	23.511	-13.058	25.376	1.00 45.71
ATOM	1085	CA	SER	1596	24.325	-14.151	24.868	1.00 45.30
MOTA	1086	CB	SER	1596	23.633	~15.495	25.124	1.00 46.19
MOTA	1087	OG	SER	1596	22.401	-15.605	24.432	1.00 44.03
MOTA	1089	C	SER	1596	24.557	-13.968	23.366	1.00 45.09
ATOM	1090	0	SER	1596	23.891	-13.156	22.707	1.00 45.03
MOTA	1091	N	SER	1597	25.475	-14.756	22.823	1.00 44.55
MOTA	1093	CA	SER	1597	25.782	-14.690	23407	1.00 45.00
MOTA	1094	CB	SER	1597	26.921	-15.643	21.065	1.00 45.60
ATOM	1095	OG	SER	1597	27.976	-15.516	22.007	1.00 54.80
MOTA	1097	С	SER	1597	24.526	-15.076	20.633	1.00 43.92
ATOM	1098	0	SER	1597	24.233	-14.498	19.577	1.00 45.51
ATOM	1099	N	LYS	1598	23.767	-16.025	21 178	1.00 39.36
ATOM	1101	CA	LYS	1598	22.551	-16.454	20.519	1.00 36.56
ATOM	1102	CR	LYS	1598	21.978	-17.715	21.147	1.00 34.93
ATOM	1103	CG	LYS	1598	21.374	-18.643	20.101	1.00 37.52
ATOM	1104	CD	LYS	1598	20.450	-19.665	20.706	1.00 34.85
MOTA	1105	CE	LYS	1598	20.054	-20.709	19.702	1.00 30.95
MOTA	1106	NZ	LYS	1598	21.219	-21.551	19.334	1.00 30.59
ATOM	1110	С	LYS	1598	21.521	-15.336	20.552	1.00 36.21
MOTA	1111	C	LYS	1598 .	20.840	-15.099	19.548	1.00 36.39
ATOM	1112	N	ASP	1599	21.447	-14.524	21.€81	1.00 33.57
MOTA	1114	CA	ASP	1599	20.520	-13.508	21.841	1.00 31.94
ATOM	1115	CB	ASP	1599	20.635	-12.898	23.238	1.00 33.82
MOTA	1116	CG	ASP	1599	20.143	-13.838	24.339	1.00 38.08
ATOM	1117	OD1		1599	20.659	-13.717	25.475	1.00 37.52
ATOM	1118	OD2		1599		-14.691	24.072	1.00 36.17
ATOM	1119	С	ASP	1599		-12.430	20.802	1.00 30.89
ATOM	1120	0	ASP	1599	19.846	-11.945	20.153	1.00 30.88
ATOM	1121	N	LEU	1600		-12.070	20.636	1.00 31.39
ATOM	1123	CA	LEU	1600		-11.050	19.666	1.00 31.55
ATOM	1124	СВ	LEU	1600		-10.695	19.845	1.00 30.47
ATOM	1125	CG	LEU	1600	24.341	-10.072	21.190	1.00 29.24
ATOM	1126	CD1		1600	25.857	-9.923	21.226	1.00 29.75
ATOM	1127	CD2		1600	23.666	-8.731	21.404	1.00 24.50
ATOM	1128	С	LEU	1600		-11.478	18.212	1.00 31.39
MOTA	1129	0	LEU	1600		-10.686	17.418	1.00 31.23
ATOM	1130	N	VAL	1601	22.439	-12.729	17.863	1.00 30.00
MOTA	1132	CA	VAL	1601		-13.231	16.518	1.00 27.94
ATOM	1133	CB	VAL	1601		-14.600	16.261	1.00 27.68
ATOM	1134	CG1		1601		-15.108	14.885	1.00 24.69
ATOM	1135	CG2		1601		-14.474	16.362	1.00 25.87
ATOM	1136	C	VAL	1601		-13.340	16.310	1.00 28.98
ATOM	1137	0	VAL	1601		-13.151	15.191	1.00 28.55
ATOM	1138	N	SER	1602	19.904	-13.635	17.382	1.00 27.64
MOTA	1140	CA	SER	1602	18.450	-13.726	17.318	1.00 27.07

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MOTA
         1141
               CB
                   SER
                         1602
                                    17.899 -14.362
                                                    18.584
                                                             1.00 29.97
 ATOM
         1142
               OG
                   SER
                         1602
                                    16.488 -14.202
                                                    18.673
                                                             1.00 38.86
 MOTA
         1144
               С
                   SER
                         1602
                                   17.864 -12.327
                                                    17.093
                                                             1.00 27.45
 ATOM
         1145
               0
                   SER
                         1602
                                   16.826 ~12.181
                                                    16.438
                                                             1.00 29.38
 ATOM
         1146
               N
                   CYS
                         1603
                                   18.504 ~11.306
                                                    17.663
                                                             1.00 25.31
 ATOM
         1148
               CA
                   CYS
                         1603
                                   18.087
                                           -9.909
                                                    17.461
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         1149
               CB
                   CYS
                         1603
                                   19.074
                                           -8.965
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 MOTA
         1150
               SG
                   CYS
                         1603
                                   18.716
                                           -7.213
                                                    18.030
                                                             0.50 11.83 PRT1
 ATOM
         1151
               C
                   CYS
                         1603
                                   18.155
                                            -9.628
                                                    15.961
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 MOTA
         1152
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                   CYS
                         1603
                                   17.175
                                            -9.238
                                                    15.329
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 MOTA
         1153
               N
                         1604
                   ALA
                                   19.340
                                           -9.833
                                                    15.398
                                                             1.00 28.35
 ATOM
         1155
               CA
                   ALA
                         1604
                                  . 19.573
                                           -9.611
                                                    13.979
                                                             1.00 28.00
ATOM
         1156
               CB
                   ALA
                         1604
                                   20.970 -10.098
                                                    13.588 _1.00._25.49
 ATOM
         1157
               C
                   ALA
                        1604
                                   18.517 -10.295
                                                    13.132
                                                            1.00 26.69
 ATOM
         1158
                   ALA
                        1604
               0
                                   17.892
                                          -9.646
                                                    12.310
                                                             1.00 31.40
 ATOM
         1159
                   TYR
               N
                        1605
                                   18.270 -11.577
                                                    13.399
                                                             1.00 26.33
 ATOM
         1161
               CA
                   TYR
                        1605
                                   17.286 -12.384
                                                    12.666
                                                             1.00 24.79
 ATOM
         1162
               CB
                   TYR
                        1605
                                   17.209 -13.771
                                                    13.300
                                                            1.00 23.42
 ATOM
         1163
               CG
                   TYR
                        1605
                                   16.132 -14.663
                                                    12.742
                                                            1.00 29.93
 ATOM
         1164
               CD1 TYR
                        1605
                                   16.281 - 15.298
                                                    11.510
                                                            1.00 30.00
 MOTA
        1165
               CE1 TYR
                        1605
                                   15.270 -16.097
                                                    10.989
                                                            1.00 32.29
 MOTA
        1166
               CD2 TYR
                        1605
                                   14.949 -14.859
                                                    13.441
                                                            1.00 32.69
 ATOM
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               CE2 TYR
                        1605
                                   13.935 -15.650
                                                    12.934
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 ATOM
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                        1605
                                   14.091 -16.266
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                                                            1.00 34.40
 ATOM
        1169
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 MOTA
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              C
                        1605
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 ATOM
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              С
                   TYR
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                                                    11.475
                                                           1.00 25.43
 MOTA
        1173
              N
                   GLN
                        1606
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 MOTA
        1175
              CA
                  GLN
                        1606
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                                                            1.00 25.47
 ATOM
        1176
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                   GLN
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 MOTA
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                        1606
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 ATOM
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 MOTA
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 ATOM
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              NE2 GLN
                        1606
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 MOTA
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                  VAL
              CA
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                                   15.120
                                           -7.430
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 ATOM
        1188
                  VAL
              CB
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                                   16.408
                                           -6.667
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 ATOM
        1189
              CG1 VAL
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 MOTA
        1190
              CG2 VAL
                        1607
                                  16.382
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                                                            1.00 17.95
 MOTA
        1191
              C
                  VAL
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                                  15.121
                                           -7.743
                                                    10.757
                                                            1.00 27.69
 MOTA
        1192
              0
                  VAL
                        1607
                                  14.406
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                                                            1.00 30.85
 MOTA
        1193
              N
                  ALA
                        1608
                                  15.902
                                           -8.749
                                                   10.355
                                                            1.00 24.59
ATOM
        1195
              CA
                  ALA
                        1608
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                                           -9.135
                                                            1.00 23.22
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MOTA
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                                                            1.00 17.65
MOTA
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                  ALA
                        1608
                                  14.579
                                           -9.589
                                                    8.492
                                                            1.00 24.5B
ATOM
        1198
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                                          -9.372
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        1199
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MOTA
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ATOM	1204	CD	ARG	1609	11.683	-13.980	10.723	1.00 32.49	
ATOM	1205	NE	ARG	1609	10.942	-14.941	9.927	1.00 34.58	
ATOM	1207	CZ	ARG	1609	10.058	-15.792	10.437	1.00 35.69	
MOTA	1208	NH1	ARG	1609	9.800	-15.790	11.740	1.00 32.47	
ATOM	1211	NH2	ARG	1609	9.468	-16.678	9.645	1.00 36.67	
ATOM	1214	С	ARG	1609	11.421	-9.518	9.008	1.00 22.96	
ATOM	1215	0	ARG	1609	10.522	-9.582	8.155	1.00 23.65	
MOTA	1216	N	GLY	1610	11.501	-8.522	9.888	1.00 20.88	
ATOM	1218	CA	GLY	1610	10.591	-7.398	9.789	1.00 21.47	
MOTA	1219	С	GLY	1610	10.822	-6.741	8.432	1.00 23.55	
ATOM	1220	0	GLY	1610	9.872	-6.452	7.688	1.00 23.53	
MOTA	1221	N	MET	1611	12.097	-6.558	8.088	1.00 24.37	
ATOM -	12:23	·CA··	MET	1611	12.488	-5.955	6.809	1.00 25.10	
ATOM	1224	CB	MET	1611	13.991	-5.686	6.801	1.00 25.47	
ATOM	1225	CG	MET	1611	14.391	-4.4.78	7.652	1.00 27.09	
ATOM	1226	SD	MET	1611	13.362	-3.000	7.330	1.00 22.57	
ATOM	1227	CE	MET	1611	13.665	-2.715	5.612	1.00 21.91	
ATOM	1228	C	MET	1611	12.090	-6.791	5.590	1.00 26.57	
ATOM	1229	0	MET	1611	11.700	-6.251	4.553	1.00 24.98	
ATOM	1230	N	GLU	1612	12.213	-8.108	5.710	1.00 27.89	
MOTA	1232	CA	GLU	1612	11.836	-9.003	4.632	1.00 26.91	
MOTA	1233	CB	GLU	1612	12.120	-10.446	5.024	1.00 26.70	
ATOM	1234	CG	GLU	1612	11.602	-11.443	4.026	1.00 29.25	
ATOM	1235	CD	GLU	1612	11.796	-12.872	4.477	1.00 31.24	
ATOM	1236		GLU	1612	11.658	-13.143	5.692	1.00 33.39	
MOTA	1237		GLU	1612	12.085	-13.733	3.617	1.00 31.91	
ATOM	1238	C	GLU	1612	10.354	-8.812	4.305	1.00 27.55	
ATOM	1239	O	GLU	1612	9.974	-8.697	3.130	1.00 30.04	
ATOM	1240	N	TYR	1613	9.518	-8.752	5.337	1.00 25.13	
ATOM	1242	CA	TYR	1613	8.092	-9.54 5	5.133	1.00 21.91	
ATOM	1243	CB	TYR	1613	7.341	-8.625	6.462	1.00 21.00	
ATOM	1244	CG	TYR	1613	5.867	-8.318	6.335	1.00 17.47	•
ATOM	1245	CD1		1613	4.969	-9.307	5.968	1.00 18.34	
ATOM	1246	CE1		1613	3.610	-9.049	5.872	1.00 18.83	
ATOM	1247	CD2		1613	5.373	-7.041	6.600	1.00 14.48	
ATOM	1248	CE2		1613	4.017	-6.761	6.502	1.00 19.67	
MOTA	1249	CZ	TYR	1613	3.137	-7.776	6.135	1.00 22.67	
MOTA MOTA	1250	ОН	TYR	1613	1.779	-7.542	6.009	1.00 21.91	
ATOM	1252 1253	C	TYR	1613	7.870	-7.170	4.504	1.00 22.06	
ATOM		O N	TYR	1613	7.125	-7.034	3.540	1.00 22.01	
ATOM	1254 1256	N CA	LEU	1614	8.541	-6.154	5.045	1.00 22.04	
ATOM	1257	CB	LEU	1614	8.400	-4.794	4.536	1.00 20.56	
ATOM	1258	CG		1614	9.219	-3.830	5.392	1.00 18.43	
ATOM	1259		LEU	1614	8.548	-3.413	6.707	1.00 15.96	
ATOM	1260	CD1 CD2		1614	9.509	-2.571	7.518	1.00 15.70	
ATOM				1614	7.255	-2.647	6.436	1.00 11.06	
ATOM	1261 1262	C	LEU	1614	8.793	-4.671	3.066	1.00 22.69	
ATOM	1263	O N	LEU	1614	8.156	-3.939	2.294	1.00 24.91	
ATOM	1265		ALA	1615	9.840	-5.397	2.684	1.00 24.55	
ATOM	1266		ALA	1615	10.333	-5.408	1.317	1.00 21.18	
ATOM	1267		ALA	1615	11.685	-6.088	1.254	1.00 18.35	
AION	140/	С	ALA	1615	9.334	-6.107	0.404	1.00 21.97	

ATOM 1268 1615 9.089 -5.642 -0.705 1.00 23.80 0 ALA ATOM 1269 N SER 1616 8.704 -7.173 0.893 1.00 22.49 ATOM 1271 SER 1616 7.722 -7.919 0.097 1.00 21.81 CA **ATOM** 1272 SER 1616 7.305 -9.179 0.831 1.00 19.78 CB MOTA 1273 SER 1616 6.382 -8.862 1.851 OG 1.00 23.88 MOTA 1275 C SER 1616 6.475 -7.071 -0.149 1.00 23.60 **ATOM** 1276 0 SER 1616 5.733 -7.277 -1.117 1.00 21.74 MOTA 1277 N LYS 1617 6.217 -6.169 0.789 1.00 25.84 MOTA 1279 LYS 1617 5.078 CA -5.280 0.705 1.00 23.96 MOTA 1280 CB LYS 1617 4.555 -4.951 2.099 1.00 20.74 ATOM 1281 CG LYS 1617 3.843 -6.124 2.750 1.00 23.40 ATOM 1282 CD LYS 1617 2.509 -6.395 2.081 1.00 28.70 1.00 31.16 **ATOM** 1283 CE LYS .1617 -7.442 2.809 1.714 -8.767 ATOM NZ 2.616 1284 LYS 1617 2.339 1.00 41.91 **ATOM** 1288 C LYS 1617 5.409 -4.019 -0.061 1.00 24.25 MOTA 1289 C LYS 1617 4.640 -3.053 -0.022 1.00 25.22 **MOTA** 1290 N 1618 6.557 ~4.028 -0.748 LYS 1.00 24.20 MOTA 1292 CA LYS 1618 7.014 -2.904 -1.582 1.00 25.15 ATOM 1293 -2.507 CB LYS 1618 5.906 -2.571 1.00 27.00 ATOM -3.411 1294 CG -3.790 LYS 1618 5.735 1.00 29.09 ATOM 1295 CD LYS 1618 5.506 - 4.864 -3.432 1.00 31.82 MOTA 1296 -5.752 CE LYS 1618 5.533 -4.663 1.00 30.21 MOTA 1297 ΝZ LYS 1618 4.231 -5.707 -5.369 1.00 26.34 -1.658 MOTA 1301 C LYS 1618 7.466 -0.816 1.00 23.50 MOTA 1302 -0.576 0 LYS 1618 7.537 -1.385 1.00 22.10 -1.821 **ATOM** 1.303 N CYS 1619 7.827 0.449 1.00 23.72 MOTA -0.693 1305 CA CYS 1619 8.213 1.275 1.00 20.89 **MOTA** -0.814 1306 CB CYS 1619 7.535 2.647 1.00 18.41 **ATOM** SG 0.405 1307 CYS 1619 8.019 3.894 1.00 26.34 **ATOM** 1308 С CYS 1619 9.717 -0.529 1.451 1.00 22.94 MOTA 1309 0 CYS 1619 10.419 -1.487 1.790 1.00 23.20 **ATOM** 1310 N ILE 1620 10.197 0.690 1.211 1.00 21.17 **ATOM** 1312 CA ILE 1620 1.039 1.388 11.610 1.00 22.35 **ATOM** 1313 CB ILE 1620 12.151 1.823 0.172 1.00 17.30 ATOM 1314 CG2 ILE 1620 2.215 0.393 1.00 8.27 13.607 **ATOM** 1315 CG1 ILE 1620 11.966 0.997 -1.111 1.00 18.27 **ATOM** 1316 CD1 ILE 1620 12.127 1.803 -2.401 1.00 17.57 **ATOM** 1317 C ILE 1620 11.631 1.926 2.652 1.00 25.20 MOTA 1318 О ILE 1620 10.912 2.932 2.715 1.00 29.69 MOTA 1.526 1319 N HIS 1621 12.398 3.665 1.00 22.66 **ATOM** 1321 CA HIS 1621 12.463 2.254 4.931 1.00 22.78 MOTA 1322 CB HIS 1621 13.214 1.425 5.980 1.00 22.65 MOTA 1323 CG HIS 1621 13.024 1.897 7.398 1.00 22.07 MOTA 1324 CD2 HIS 1621 12.485 1.280 8.475 1.00 20.50 ATOM 1325 ND1 HIS 1621 13.449 3.134 7.842 1.00 23.11 MOTA 1327 CE1 HIS 1621 13.182 3.253 9.131 1.00 23.92 MOTA 1328 NE2 HIS 1621 12.596 2.144 9.543 1.00 24.44 MOTA 1330 C HIS 1621 13.110 3.616 4.831 1.00 24.07 MOTA 1331 HIS 1621 12.561 4.597 0 5.306 1.00 24.37 ATOM 1332 N ARG 1622 14.327 3.639 4.291 1.00 26.42 **ATOM** 1334 CA ARG 1622 15.129 4.853 4.130 1.00 24.59 ATOM 1335 CB ARG 1622 14.289 6.018 3.581 1.00 17.58

ATOM	1336	CG	ARG	1622	13.810	5.767	2.163	1.00 13.88	
ATOM	1337	CD	ARG	1622	12.925	6.860	1.634	0.50 4.97	
ATOM	1338	NE	ARG	1622	12.574	6.590	0.243	0.50 6.49	
MOTA	1340	CZ	ARG	1622	11.537	5.852	-0.145	0.50 3.84	
ATOM	1341	NH1	ARG	1622	10.719	5.308	0.753	0.50 2.25	
MOTA	1344	NH2	ARG	1622	11.356	5.611	-1.433	0.50 2.48	
MOTA	1347	С	ARG	1622	15.918	5.257	5.388	1.00 24.72	
ATOM	1348	0	ARG	1622	16.767	6.138	5.337	1.00 26.90	
ATOM	1349	N	ASP	1623	15.685	4.585	6.505	1.00 25.61	
MOTA	1351	CA	ASP	1623	16.437	4.927	7.703	1.00 28.41	
ATOM	1352	CB	ASP	1623	15.922	6.213	8.349	1.00 30.38	
ATOM	1353	CG	ASP	1623	16.891	6.772	9.373	1.00 33.47	
MOTA	1354	OD1	ASP -	-1623	16.428	7.338	10.382	1.00 43.35	
ATOM	1355	OD2	ASP	1623	18.121	6.645	9.167	1.00 31.88	
MOTA	1356	С	ASP	1623	16.498	3.797	8.713	1.00 28.86	
MOTA	1357	0	ASP	1623	16.148	3.959	9.887	1.00 28.31	
MOTA	1358	N	LEU	1624	16.956	2.642	8.246	1.00 27.81	
MOTA	1360	CA	LEU	1624	17.087	1.480	9.107	1.00 27.28	
MOTA	1361	CB	LEU	1624	17.149	0.220	8.242	1.00 27.53	
MOTA	1362	CC	LEU	1624	17.118	-1.150	8.916	1.00 27.69	
ATOM.	1363	CD1	LEU	1624	15.850	-1.348	9.756	1.00 23.77	
MOTA	1364	CD2	LEU	1624	17.228	-2.175	7.805	1.00 29.15	
ATOM	1365	C	LEU	1624	18.340	1.628	10.002	1.00 26.27	
MOTA	1366	0	LEU	1624	19.464	1.773	9.514	1.00 25.89	
ATOM	1367	N	ALA	1625	18.116	1.598	11.313	1.00 23.29	
MOTA	1369	CA	ALA	1625	19.164	1.750	12.314	1.00 19.68	
MOTA	1370	CB	ALA	1625	19.520	3.233	12.473	1.00 18.85	
MOTA	1371	C	ALA	1625	18.575	1.214	13.613	1.00 20.79	
MOTA	1372	0	ALA	1625	17.352	1.077	13.716	1.00 20.75	
MOTA	1373	N	ALA	1626	19.429	0.942	14.605	1.00 22.03	
MOTA	1375	CA	ALA	1626	18.969	0.408	15.900	1.00 23.43	
MOTA	1376	CB	ALA	1626	20.139	-0.048	16.764	1.00 22.46	
ATOM	1377	C	ALA	1626	18.111	1.397	16.664	1.00 25.86	
MOTA	1378	0	ALA	1626	17.333	1.006	17.523	1.00 29.51	
MOTA	1379	N	ARG	1627	18.303	2.685	16.407	1.00 26.92	
MOTA	1381	CA	ARG	1627	17.503	3.722	17.048	1.00 27.30	
ATOM	1382	CB	ARG	1627	18.017	5.107	16.627	1.00 28.29	
ATOM	1383	CG	ARG	1627	18.086	5.287	15.104	1.00 36.26	
ATOM	1384		ARG	1627	18.255	6.756	14.688	1.00 41.19	
ATOM	1385	NE	ARG	1627	18.548	6.928	13.261	1.00 39.94	
ATOM	1387	CZ	ARG	1627	19.779	6.904	12.749	1.00 42.33	
ATOM	1388	NH1		1627	20.826	6.721	13.539	1.00 44.75	
ATOM	1391	NH2		1627	19.976	7.059	11.450	1.00 41.50	
MOTA	1394	C	ARG	1627	16.029	3.567	16.591	1.00 27.42	
ATOM	1395	0	ARG	1627	15.092	3.897	17.333	1.00 26.53	
ATOM	1396	N	ASN	1628	15.850	3.039	15.375	1.00 26.82	
ATOM	1398	CA	ASN	1628	14.534	2.849	14.758	1.00 24.08	
MOTA	1399	CB	ASN	1628	14.569	3.308	13.301	1.00 26.30	
MOTA	1400	CG	ASN	1628	14.709	4.823	13.167	1.00 25.19	
MOTA	1401	OD1		1628	14.018	5.567	13.844	1.00 28.59	
ATOM	1402	ND2		1628	15.599	5.277	12.297	1.00 22.32	
ATOM	1405	С	ASN	1628	13.945	1.440	14.862	1.00 24.35	

MOTA	1406	0	ASN	1628	13.026	1.084	14.105	1.00 24.66
ATOM	1407	И	VAL	1629	14.473	0.637	15.785	1.00 22.35
MOTA	1409	CA	VAL	1629	13.988	-0.718	16.055	1.00 20.65
MOTA	1410	CB	VAL	1629	15.077	-1.813	15.822	1.00 18.07
ATOM	1411	CG1	VAL	1629	14.612	-3.142	16.398	1.00 11.84
MOTA	1412		VAL	1629	15.378	-1.977	14.346	1.00 12.65
MOTA	1413	C	VAL	1629	13.625	-0.670	17.536	1.00 24.27
ATOM	1414	0	VAL	1629	14.427	-0.237	18.361	1.00 25.94
ATOM	1415	N	LEU	1630	12.393	-1.031	17.866	1.00 24.99
MOTA	1417	CA	LEU	1630	11.936	-1.010	19.247	1.00 25.50
MOTA	1418	CB	LEU	1630	10.609	-0.252	19.339	1.00 22.79
MOTA	1419	CG	LEU	1630	10.634	1.179	18.789	1.00 17.86
ATOM	1420	CD1	LEU	1630	9.240	1 680	18.654	1.00 18.49
ATOM	1421	CD2	LEU	1630	11.409	2.100	19.668	1.00 17.63
ATOM	1422	C	LEU	1630	11.833	-2.434	19.829	1.00 28.29
ATOM	1423	0	LEU	1630	11.666	-3.412	19.092	1.00 28.56
ATOM	1424	N	VAL	1631	11.933	-2.542	21.150	1.00 29.46
MOTA	1426	CA	VAL	1631	11.883	-3.831	21.833	1.00 29.40
MOTA	1427	CB	VAL	1631	13.222	-4.105	22.553	1.00 27.48
ATOM	1428	CG1	VAL	1631	13.210	-5.477	23.233	1.00 24.53
MOTA	1429	€G2	VAL	1631	14.376	-3.976	21.576	1.00 22.55
MOTA	1430	С	VAL	1631	10.730	-3.918	22.853	1.00 31.94
ATOM	1431	0	VAL	1631	10.630	-3.102	23.787	1.00 33.13
ATOM	1432	И	THR	1632	9.866	-4.911	22.559	1.00 32.21
ATOM	1434	$\mathbb{C}\mathbf{A}$	'l'HR	1632	8.728	-5.149	23.540	1.00 31.77
ATOM	1435	CB	THR	1632	7.674	6.061	22.374	1.00 32.38
ATOM	1436	OG1	THR	1632	8.169	-7.406	22.792	1.00 32.36
ATOM	1438	CG2	THR	1632	7.330	. 5.554	21.480	1.00 28.05
ATOM	1439	C	THR	1632	9.157	-5.810	24.842	1.00 30.39
.ATOM	1440	Ċ.	THR	1632	10.256	-6.320	24.947	1.00 30.28
MOTA	1441	N	GLU	1633	8.260	-5.823	25.822	1.00 32.43
ATOM	1443	CA	GLU	1633	8.513	-6.424	27.122	1.00 32.84
ATOM	1444	CB	GLU	1633	7.259	-6.310	27.991	1.00 35.28
ATOM	1.445	CG	GLU	1633	7.386	-6.881	29.399	1.00 46.57
ATOM	1446	CD	GLU	1633	8.463	-6.192	30.260	1.00 54.03
ATOM	1447		GLU	1633	8.519	-4.939	30.297	1.00 58.68
ATOM	1448		GLU	1633	9.249	-6.916	30.918	1.00 56.84
MOTA	1449	С	GLU	1633	8.914	-7.889	26.986	1.00 35.14
ATOM	1450	0	GLU	1633	9.632	-8.435	27.826	1.00 33.92
ATOM	1451	N	ASP	1634	8.456	-8.526	25.910	1.00 38.25
ATOM	1453	CA	ASP	1634		-9.941	25.677	1.00 39.22
ATOM	1454	СВ	ASP	1634		-10.639	24.990	1.00 44.88
ATOM	1455	CG	ASP	1634		-10.420	25.725	1.00 54.17
ATOM	1456	OD1		1634		-11.042	26.799	1.00 56.33
ATOM	1457	OD2		1634	5.412	-9.622	25.236	1.00 54.47
ATOM	1458	С	ASP	1634		-10.109	24.849	1.00 37.53
ATOM	1459	0	ASP	1634		-11.225	24.495	1.00 36.33
MOTA	1460	N	ASN	1635	10.730	-8.998	24.589	1.00 39.12
ATOM	1462	CA	ASN	1635	11.974	-8.948	23.792	1.00 37.21
ATOM	1463	CB	ASN	1635	13.042	-9.891	24.361	1.00 37.83
ATOM	1464	CG	ASN	1635	13.576	-9.426	25.677	1.00 38.65
ATOM	1465	OD1	ASN	1635	13.795	-8.236	25.880	1.00 43.82

ATOM	1466	ND2	ASN	1635	13.768	-10.353	26.596	1.00	39.49
ATOM	1469	C	ASN	1635	11.807	-9.193	22.287	1.00	35.03
ATOM	1470	0	ASN	1635	12.649	-9.834	21.648	1.00	32.37
ATOM	1471	N	VAL	1636	10.705	-8.700	21.736	1.00	33.30
ATOM	1473	CA	VAL	1636	10.418	-8.846	20.320	1.00	30.50
ATOM	1474	CB	VAL	1636	8.895	-9.014	20.075	1.00	31.54
ATOM	1475	CG1	VAL	1636	8.600	-9.178	18.584	1.00	29.16
ATOM	1476	CG2	VAL	1636	8.384	-10.214	20.838	1.00	34.29
ATOM	1477	С	VAL	1636	10.908	-7.577	19.629	1.00	29.28
ATOM	1478	0	VAL	1636	10.553	-6.463	20.037	1.00	27.08
ATOM	1479	N	MET	1637	11.760	-7.755	18.623	1.00	27.82
ATOM	1481	CA	MET	1637	12.318	-6.634	17.874	1.00	27.09
ATOM	1482	CB	MET	1637	13.578	-7.070	17.127	1.00	27.47
MOTA	1483	CG	MET	1637	14.648	-7.697	18.010	1.00	28.35
ATOM	1484	SD	MET	1637	15.243	-6.594	19.297	1.00	30.41
ATOM	1485	CE	MET	1637	15.104	-7.640	20.728	1.00	26.00
ATOM	1486	C	MET	1637	11.272	-6.200	16.868	1.00	26.01
ATOM	1487	0	MET	1637	10.751	-7.034	16.131	1.00	26.05
ATOM	1488	N	LYS	1638	10.983	4.900	16.823	1.00	25.44
ATOM	1490	CA	LYS	1638	9.984	-4.349	15.906	1.00	22.01
ATOM	1491	CB	LYS	1638	8.693	-4.028	16.658	1.00	19.65
ATOM	1492	CG	LYS	1638	7.887	-5.254	17.034	1.00	21.22
ATOM	1493	CD	LYS	1638	6.666	-4.904	17.869	1.00	21.73
ATOM	1494	CE	LYS	1638	5.776	-6.133	18.076	1.00	19.32
ATOM	1495	NZ	LYS	1638	4.970	· 5 . 522	16.869	1.00	23.14
ATOM	1499	С	LYS	1638	10.477	-3.106	15.191	1.00	21.85
ATOM	1500	0	LYS	1638	10.896	-2.147	15.808	1.00	24.35
ATOM	1501	N	ILE	1639	10.371	.3.110	13.878	1.00	24.47
ATOM	1503	CA	ILE	1639	10.803	-1.983	13.073	1.00	24.90
ATOM	1504	CB	ILE	1639	11.090	-2.443	11.625	1.00	22.12
ATOM	1505	CG2	ILE	1639	11.413	-1.275	10.720	1.00	17.41
MOTA	1506	CG1	ILE	1639	12.256	-3.423	11.664	1.00	18.67
ATOM	1507	CD1	ILE	1639	12.309	-4.308	10.492	1.00	26.15
ATOM	1508	C	ILE	1639	9.772	-0.856	13.117		28.52
ATOM	1509	0	ILE	1639	8.557	-1.094	12.964	ι.00	
ATOM	1510	N	ALA	1640	10.267	0.363	13.358	1.00	30.06
ATOM	1512	CA	ALA	1640	9.444	1.564	13.445	1.00	29.37
ATOM ATOM	1513	CB	ALA	1640	9.627	2.211	14.812		28.25
	1514	C	ALA	1640	9.782	2.566	12.344		29.68
ATOM	1515	0	ALA	1640	10.808	2.453	11.660		30.81
ATOM ATOM	1516 1518	N	ASP	1641	8.892	3.536	12.154	1.00	
ATOM		CA	ASP	1641	9.067	4.608	11.154	1.00	
ATOM	1519 1520	CB	ASP	1641	10.309	5.454	11.454	1.00	
ATOM	1521	CG	ASP	1641	10.018	6.678	12.321	1.00	
ATOM		OD1		1641	10.952	7.497	12.469	1.00	
ATOM	1522	OD2		1641	8.897	6.824	12.856	1.00	
ATOM	1523		ASP	1641	9.102	4.162	9.705	1.00	
	1524	0	ASP	1641	9.484	4.941	8.826	1.00	
ATOM	1525	N	PHE	1642	8.650	2.941	9.440	1.00	
ATOM ATOM	1527	CA	PHE	1642	8.648	2.435	8.072	1.00	
ATOM	1528	CB	PHE	1642	8.432	0.909	8.043	1.00	
AION	1529	CG	PHE	1642	7.135	0.451	8.639	1.00	16.47

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ATOM 1530 CD1 PHE 1642 5.974 0.400 7.878 1.00 21.72 **ATOM** CD2 PHE 1531 1642 7.080 0.018 9.945 1.00 17.01 **ATOM** 1532 CE1 PHE 1642 4.781 -0.082 8.422 1.00 20.97 ATOM 1533 CE2 PHE 1642 5.892 -0.463 10.496 1.00 18.72 **ATOM** 1534 CZPHE 1642 4.743 -0.515 9.739 1.00 20.32 **ATOM** 1535 C PHE 1642 7.667 3.174 7.157 1.00 25.57 **ATOM** 1536 0 PHE 1642 7.910 3.292 5.971 1.00 28.40 MOTA 1537 GLY N 1643 6.585 3.718 7.707 1.00 25.69 MOTA 1539 CA GLY 1643 5.631 4.427 6.866 1.00 24.81 MOTA 1540 C GLY 1643 5.786 5.935 6.893 1.00 24.84 MOTA 1541 О GLY 1643 4.922 6.684 6.436 1.00 19.20 MOTA 1542 N LEU 1644 6.930 6.387 7.376 1.00 29.50 MOTA 1544 CA LEU 1644 7.189 7.808. 7.491, 1.00 34.24 **ATOM** 1545 CB LEU 1644 8.498 8.037 8.242 1.00 33.10 **ATOM** 1546 CG LEU 1644 8.473 9.371 8.962 1.00 36.00 **ATOM** 1547 CD1 LEU 1644 7.520 9.212 10.127 1.00 41.52 **ATOM** 1548 CD2 LEU 1644 9.854 9.773 9.442 1.00 35.23 ATOM 1549 C LEU 1644 7.213 8.578 6.179 1.00 37.54 ATOM: 1550 0 LEU 1644 7.759 8.123 5.176 1.00 37.48 MOTA 1551 N ALA 1645 6.577 9.744 6.203 1.00 41.66 MOTA 1553 CA ALA 1645 6.524 10.652 5.067 1.00 43.66 ATOM 1554 CB ALA 1645 5.309 11.563 5.202 1.00 38.13 ATOM 1555 C ALA 1645 7.819 11.475 5.141 1.00 44.67 **ATOM** 1556 0 ALA 1645 8.105 12.082 6.176 1.00 47.17 MOTA 1557 1.00 45.69 N ALA 1646 8.622 11.462 4.082 ATOM 1559 CA ALA 1646 9.871 12.222 4.094 1.00 48.62 **ATOM** 1560 ALA CB 1646 10.971 11.405 4.778 1.00 49 50 MOTA 1561 C ALA 1646 10.338 12.661 2.712 1.00 50.98 ATOM 1562 0 ALA 1646 10.319 11.880 1.759 1.00 52.84 ATOM 1563 N ASP 1647 10.755 13.919 2.598 1.00 53.09 MOTA 1565 CA ASP 1647 11.253 14.419 1.322 1.00 55.06 **ATOM** 1566 CB ASP 1647 15.887 10.868 1.092 1.00 56.05 MOTA 1567 CG ASP 1647 11.084 16.342 -0.352 1.00 59.31 MOTA 1568 OD1 ASP 1647 12.070 15.928 -1.003 1.00 59.51 MOTA 1569 OD2 ASP 1647 10.265 17.150 -0.837 1.00 63.48 ATOM 1570 C ASP 1647 12.770 14.264 1.332 1.00 55.26 **ATOM** 1571 ASP О 1647 13.487 15.075 1.926 1.00 53.18 **ATOM** 1572 N ILE 1648 13.235 13.198 0.684 1.00 56.66 **ATOM** 1574 CA ILE 1648 14.652 1.00 57.79 12.877 0.595 ATOM 1575 CB ILE 1648 14.890 11.624 -0.271 1.00 53.86 **ATOM** 1576 ILE CG2 1648 14.133 10.443 0.326 1.00 52.14 MOTA 1577 CG1 ILE 1648 14.454 11.886 -1.718 1.00 48.24 MOTA 1578 CD1 ILE 1648 15.198 11.083 -2.751 1.00 43.97 **MOTA** 1579 C ILE 1648 15.439 14.044 -- 0.014 1.00 62.32 **ATOM** 1580 0 1648 ILE 16.591 14.271 0.380 1.00 64.72 **ATOM** 1581 N HIS 1649 14.805 14.791 -0.884 1.00 65.72 ATOM 1583 CA HIS 1649 15.450 15.941 -1.500 1.00 69.00 ATOM 1584 CB HIS 1649 14.793 -2.844 16.285 1.00 70.35 ATOM 1585 CG HIS 1649 15.123 15.332 -3.944 1.00 73.90 ATOM 1586 CD2 HIS 1649 16.257 14.628 -4.208 1.00 75.13 MOTA 1587 ND1 HIS 1649 14.239 15.006 -4.946 1.00 75.30 ATOM 1589 CE1 HIS 1649 14.798 14.148 -5.779 1.00 76.83

ATOM	1590	NE2	HIS	1649	16.025	13.905	-5.348	1.00 76.74
MOTA	1592	С	HIS	1649	15.419	17.150	-0.576	1.00 70.22
ATOM	1593	0	HIS	1649	15.517	18.284	-1.041	1.00 72.83
MOTA	1594	N	HIS	1650	15.218	16.912	0.718	1.00 71.28
MOTA	1596	CA	HIS	1650	15.199	17.987	1.710	1.00 72.52
ATOM	1597	CB	HIS	1650	13.776	18.488	1.956	1.00 75.67
ATOM	1598	CG	HIS	1650	13.272	19.401	0.882	1.00 82.16
MOTA	1599	CD2	HIS	1650	13.451	20.734	0.691	1.00 86.17
MOTA	1600	ND1	HIS	1650	12.529	18.955	-0.185	1.00 86.37
ATOM	1602	CE1	HIS	1650	12.262	19.972	-0.993	1.00 89.04
ATOM	1603	NE2	HIS	1650	12.814	21.058	-0.481	1.00 89.37
ATOM	1605	C	HIS	1650	15.856	17.593	3.029	1.00 71.11
ATOM	1606	0	HIS	1650	15.783	18.334	4.010	1.00 69.56
MOTA	1607	N	ILE	1651	16.543	16.451	3.033	1.00 70.84
MOTA	1609	CA	ILE	1651	17.221	15.939	4.222	1.00 70.50
MOTA	1610	CB	ILE	1651	17.622	14.462	4.031	1.00 71.73
ATOM	1611	CG2	ILE	1651	18.499	13.978	5.194	1.00 71.65
MOTA	1612	CG1	ILE	1651	16.359	13.604	3.890	1.00 73.10
MOTA	1613	CD1	ILE	1651	16.643	12.143	3.593	1.00 75.18
MOTA	1614	C	ILE	1651	18.472	16.734	4.569	1.00 69.85
ATOM	1615	0	ILE	1651	19.375	. 16.882	3.745	1.00 70.30
ATOM	1616	N	ASP	1652	18.543	17.222	5.802	1.00 68.99
MOTA	1618	CA	ASP	1652	19.707	17.987	6.240	1.00 68.06
ATOM	1619	CB	ASP	1652	19.344	18.923	7 398	1.00 70.53
MOTA	1620	CG	ASP	1652	20.512	19.790	7.843	i.00 72.86
ATOM	1621	OD1	ASP	1652	21.306	20.248	6.985	1.00 73.36
MOTA	1622	OD2	ASP	1652	20.646	20.034	9.060	1.00 76.01
ATOM	1623	С	ASP	1652	20.802	17.023	5.673	1.00 66.08
MOTA	1624	0	ASP	1652	20.746	16.457	7.762	1.00 64.92
ATOM	1625	N	TYR	1653	21.802	16.856	5.814	1.00 64.14
ATOM	1627	CA	TYR	1653	22.926	15.968	6.089	1.00 63.02
MOTA	1628	CB	TYR	1653	23.852	15.906	4.875	1.00 61.29
ATOM	1629	CG	TYR	1653	23.362	14.971	3.795	1.00 62.37
ATOM	1630	CD1		1653	24.153	14.679	2.684	1.00 61.11
ATOM	1631	CE1	TYR	1653	23.725	13.773	1.717	1.00 62.89
ATOM	1632	CD2	TYR	1653	22.121	14.335	3.910	1.00 64.11
ATOM	1633		TYR	1653	21.685	13.429	2.953	1.00 66.09
ATOM	1634	CZ	TYR	1653	22.487	13.148	1.859	1.00 65.03
ATOM	1635	OH	TYR	1653	22.044	12.239	0.921	1.00 65.78
ATOM	1637	С	TYR	1653	23.733	16.313	7.345	1.00 63.49
ATOM	1638	0	TYR	1653	24.403	15.453	7.912	1.00 63.39
ATOM	1639	N	TYR	1654	23.644	17.564	7.789	1.00 64.37
ATOM	1641	CA	TYR	1654	24.379	18.013	8.963	1.00 63.95
MOTA	1642	CB	TYR	1654	24.947	19.417	8.741	1.00 60.86
ATOM	1643	CG	TYR	1654	26.038	19.467	7.691	1.00 57.70
ATOM	1644	CD1		1654	25.736	19.698	6.353	1.00 58.03
ATOM	1645	CE1		1654	26.734	19.708	5.383	1.00 60.65
ATOM	1646	CD2		1654	27.364	19.252	8.035	1.00 56.79
ATOM	1647	CE2		1654	28.366	19.261	7.079	1.00 58.85
ATOM	1648	CZ	TYR	1654	28.047	19.488	5.754	1.00 60.88
ATOM	1649	OH	TYR	1654	29.048	19.485	4.806	1.00 64.23
MOTA	1651	C	TYR	1654	23.560	17.980	10.239	1.00 65.89

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MOTA 1652 TYR 1654 18.283 11.316 1.00 67.56 0 24.074 N **ATOM** 1653 LYS 1655 17.586 10.135 22.297 1.00 67.36 ATOM 1655 CA LYS 1655 21.443 17.527 11.315 1.00 69.11 ATOM 1656 CB LYS 19.972 17.611 10.915 1655 1.00 69.86 MOTA 1657 CG LYS 1655 19.019 17.651 12.090 1.00 71.45 **ATOM** 1658 LYS 17.607 CD1655 17.867 11.603 1.00 75.40 ATOM 1659 CE LYS 1655 16.595 17.393 12.627 1.00 78,22 **ATOM** 1660 NZ LYS 15.204 17.553 1655 12.110 1.00 80.61 MOTA 1664 С LYS 1655 21.714 16.242 12.093 1.00 69.65 ATOM 1665 0 LYS 1655 21.872 15.169 11.497 1.00 70.67 **ATOM** 1666 N LYS 1656 21.766 16.358 13.419 1.00 68.19 **ATOM** 1668 CA LYS 1656 22.035 15.212 14.275 1.00 68.00 MOTA 1669__CB LYS 1656 22.983 15.618 15.403 1.00.65.53 MOTA 1670 CG LYS 1656 24.395 15.895 14.946 1.00 62.71 **ATOM** 1671 CDLYS 1656 25.280 16.221 16.138 1.00 64.38 **ATOM** 1672 CE LYS 1656 26.764 16.031 15.832 1.00 63.23 **ATOM** 1673 NZ LYS 1656 27.592 16.186 17.062 1.00 61.72 MOTA 1677 C LYS 1656 20.777 14.560 14.855 1.00 68.73 **ATOM** 1678 0 LYS 1656 19.695 15 148 14.837 1.00 69.20 **ATOM** 1679 THR N 1657 20.928 13.337 15.359 1.00 68.48 **ATOM** 1681 CA THR 1657 19.821 12.607 15.960 1.00 67.93 **ATOM** 1682 CB THR 1657 20.109 11.078 16.021 1.00 68.93 **ATOM** 1683 OG1 THR 1657 21.295 1.00 68.72 10.823 16.787 MOTA 1685 CG2 THR 1657 20.289 10.500 14.637 1.00 68.83 **ATOM** 1686 C THR 1657 19.682 13.131 17.383 1.60 67.80 ATOM 1687 0 THR 20.424 1657 14.022 17.790 1.00 67.87 MOTA 1688 N ALA 1658 18.753 12.569 18.148 1.00 68.95 ATOM 1690 CA ALA 18.580 1658 12.992 19.537 1.00 70.64 MOTA 1691 CB ALA 1658 17.391 12.254 20.173 1.00 71.19 **ATOM** 1692 C ALA 1658 19.880 12.709 20.313 1.00 69.64 **ATOM** 1693 ALA 20.394 0 1658 13.566 21.042 1.00 70.13 ATOM 1694 Ŋ ASN 1659 20.440 11.526 20.080 1.00 68.02 ATOM 1696 CA ASN 21.663 1659 11.092 20.746 1.00 66.10 MOTA 1697 CB ASN 21.835 1659 9.583 20.557 1.00 70.23 MOTA 1698 CG ASN 22.632 8.937 1.00 74.09 1659 21.679 **ATOM** 1699 OD1 ASN 1659 22.525 9.331 22.840 1.00 75.21 MOTA 1700 ND2 ASN 1659 23.402 7.907 21.342 1.00 75.03 MOTA 1703 С ASN 1659 22.910 11.816 20.249 1.00 63.30 ATOM 1704 0 ASN 1659 24.004 11.585 20.762 1.00 61.12 ATOM 1705 N GLY 22.744 1660 12.678 19.246 1.00 61.61 ATOM 1707 CA GLY 23.867 1660 13.421 18.689 1.00 59.06 ATOM 170B С GLY 1660 24.604 12.750 17.536 1.00 56.84 ATOM 1709 0 GLY 1660 25.726 13.132 17.196 1.00 55.69 MOTA 1710 .N ARG 23.980 1661 11.758 16.914 1.00 55.73 **ATOM** 1712 CA ARG 1661 24.626 11.062 15.808 1.00 52.76 ATOM 1713 CB ARG 1661 24.387 9.549 15.883 1.00 52.39 **ATOM** 1714 CG ARG 1661 24.977 8.874 17.111 1.00 54.08 **ATOM** 1715 CD ARG 1661 24.776 7.376 17.045 1.00 58.37 MOTA 1716 NE ARG 1661 25.178 6.665 18.260 1.00 59.27 MOTA 1718 CZARG 1661 24.952 5.369 18.471 1.00 59.83 MOTA 1719 NH1 ARG 1661 24.319 4.643 17.550 1.00 57.04 MOTA 1722 NH2 ARG 1661 25.375 4.792 19.591 1.00 59.47

ATOM	1725	C	ARG	1661	24.167	11609	14.468	1.00 49.58
ATOM	1726	0	ARG	1661	23.169	12.321	14.375	1.00 47.38
ATOM	1727	N	LEU	1662	24.911	11.266	13.430	1.00 46.26
ATOM	1729	CA	LEU	1662	24.600	11.717	12.092	1.00 44.75
ATOM	1730	CB	LEU	1662	25.871	12.261	11.425	1.00 43.49
ATOM	1731	CG	LEU	1662	26.430	13.561	12.020	1.00 43.01
ATOM	1732	CD1	LEU	1662	27.918	13.705	11.727	1.00 42.40
ATOM	1733	CD2	LEU	1662	25.644	14.760	11.507	1.00 40.19
ATOM	1734	С	LEU	1662	23.999	10.570	11.276	1.00 43.58
ATOM	1735	0	LEU	1662	24.704	9.628	10.892	1.00 43.68
MOTA	1736	N	PRO	1663	22.680	10.631	11.010	1.00 40.72
MOTA	1737	CD	PRO	1663	21.723	11.629	11.521	1.00 40.27
ATOM	1738	C'A	PRO -	1663	21.981	9.603	10.237	1.00 36.86
ATOM	1739	CB	PRO	1663	20.595	10.214	10 035	1.00 36.67
ATOM	1740	CG	PRO	1663	20.375	10.937	11.314	1.00 36.84
ATOM	1741	С	PRO	1663	22.640	9.266	8.907	1.00 33.34
MOTA	1742	O	PRO	1663	22.442	8.161	8.401	1.00 33.65
ATOM	1743	N	VAL	1.664	23.427	10.188	8.343	1.00 31.26
ATOM	1745	CA	VAL	1664	24.095	9.915	7.058	1.00 30.43
ATOM	1746	CE	VAL	1664	24.887	11.125	6.46€	1.00 27.09
ATOM	1747	CG1	VAL	1664	23.947	12.199	6.040	1.00 23.98
MOTA	1748	CG2	VAL	1664	25.894	11.654	7.464	1.00 26.06
MOTA	1749	C	VAL	1664	25.044	8.728	7.163	1.00 28.18
ATOM	1750	0	VAL	1664	25.461	8.178	6.153	1.00 28.30
ATOM	1751	N	LYS	1665	25.353	8.326	8.389	1.00 25.52
ATOM	1753	CA	LYS	1665	26.243	7.200	8.612	1.00 25.48
ATOM	1754	CB	LYS	1665	26.915	7.334	9.979	1.00 23.52
ATOM	1755	CG	LYS	1665	27.910	8.452	10.001	1.00 23.14
ATOM	1756	CD	LYS	1665	28.363	8.776	11.400	1.00 29.84
MOTA	1757	CE	LYS	1665	29.430	9.871	11.385	1.00 28.33
ATOM	1758	NZ	LYS	1665	29.794	10.283	12.777	1.00 30.88
ATOM	1762	C	LYS	1665	25.595	5.823	8.413	1.00 25.26
ATOM	1763	0	LYS	1665	26.261	4.798	8.512	1.00 23.05
ATOM	1764	N	TRP	1666	24.289	5.815	8.156	1.00 27.05
ATOM	1766	CA	TRP	1666	23.543	4.588	7.884	1.00 27.17
ATOM	1767	CB	TRP	1666	22.282	4.529	8.760	1.00 26.98
ATOM	1768	CG	TRP	1666	22.563	4.067	10.197	1.00 29.62
ATOM	1769	CD2		1666	23.065	4.857	11.283	1.00 29.64
ATOM ATOM	1770	CE2	TRP	1666	23.230	3.988	12.393	1.00 28.25
	1771	CE3	TRP	1666	23.406	6.208	11.430	1.00 29.15
ATOM ATOM	1772	CD1		1666	22.436	2.793	10.690	1.00 26.48
ATOM	1773	NE1		1666	22.834	2.737	11.997	1.00 24.81
ATOM	1775 1776	CZ2		1666	23.719	4.430	13.636	1.00 28.40
ATOM				1666	23.894	6.647	12.670	1.00 29.38
	1777		TRP	1666	24.048	5.756	13.749	1.00 29.83
ATOM	1778	C	TRP	1666	23.176	4.499	6.385	1.00 27.71
ATOM	1779	0	TRP	1666	22.745	3.451	5.900	1.00 29.42
MOTA	1780	N	MET	1667	23.439	5.572	5.645	1.00 25.52
ATOM	1782	CA	MET	1667	23.098	5.642	4.232	1.00 25.24
ATOM	1783	CB	MET	1667	22.972	7.095	3.792	1.00 26.58
ATOM	1784		MET	1667	21.830	7.836	4.391	1.00 32.35
ATOM	1785	SD	MET	1667	21.846	9.559	3.8 7 7	1.00 40.32

ATOM	1786	CE	MET	1667	21.033	9.447	2.341	1.00 38.17
ATOM	1787	С	MET	1667	24.042	4.960	3.276	1.00 25.07
ATOM	1788	0	MET	1667	25.256	5.037	3.411	1.00 27.61
ATOM	1789	N	ALA	1668	23.473	4.302	2.282	1.00 24.92
ATOM	1791	CA	ALA	1668	24.272	3.647	1.271	1.00 26.92
ATOM	1792	CB	ALA	1668	23.397	2.720	0.425	1.00 25.09
MOTA	1793	С	ALA	1668	24.866	4.759	0.410	1.00 27.82
MOTA	1794	0	ALA	1668	24.254	5.817	0.242	1.00 27.06
ATOM	1795	N	PRO	1669	26.050	4.530	-0.170	1.00 27.84
ATOM	1796	CD	PRO	1669	26.912	3.339	-0.107	1.00 27.12
MOTA	1797	CA	PRO	1669	26.662	5.561	-1.005	1.00 28.04
MOTA	1798	CB	PRO	1669	27.868	4.835	-1.593	1.00 26.71
ATOM	1799	CG	PRO	1669	28.249	3.893	-0.498	1.00 27.49
MOTA	1800	C	PRO	1669	25.734	6.078	-2.108	1.00 28.51
MOTA	1801	0	PRO	1669	25.685	7.281	-2.371	1.00 30.64
ATOM	1802	N	GLU	1670	24.992	5.179	-2.746	1.00 28.25
ATOM	1804	CA	GLU	1670	24.095	5.584	-3.826	1.00 26.82
MOTA	1805	CB	GLU	1670	23.600	4.369	-4.620	1.00 29.32
ATOM	1806	CG	GLU	1670	22.604	3.486	-3.889	1.00 30.38
ATOM	1807	CD	GLU	1670	23.223	2.266	-3.229	1.00 32.52
ATOM	1808		GLU	1670	22.444	1.393	-2.794	1.00 28.06
MOTA	1809	OE2	GLU	1670	24.474	2.175	-3.130	1.00 28.67
MOTA	1810	C.	GLU	1670	22.924	6.440	-3.356	1.00 24.79
ATOM	1811	0	GLU	1670	22.410	7.236	-4.123	1.00 22.31
ATOM	1812	N	ALA	1671	22.512	6.265	-2.101	1.00 26.70
ATOM	1814	CA	ALA	1671	21.423	7.040	-1.490	1.00 25.67
MOTA	1815	CB	ALA	1671	20.813	6.292	-0.312	1.00 18.88
MOT'A	1816	C	ALA	1671	21.984	8.365	-1.006	1.00 26.05
ATOM	1817	0	ALA	1671	21.400	9.414	-1.229	1.00 28.14
MOTA	1818	N	LEU	1672	23.138	8.300	-0.358	1.00 29.03
ATOM	1820	CA	LEU	1672	23.807	9.481	0.172	1.00 34.07
ATOM	1821	CB	LEU	1672	25.030	9.064	0.986	1.00 34.45
ATOM	1822	CG	LEU	1672	25.870	10.157	1.648	1.00 39.50
ATOM	1823		LEU	1672	25.081	10.853	2.740	1.00 41.71
ATOM	1824		LEU	1672	27.123	9.530	2.243	1.00 40.16
ATOM	1825	C	LEU	1672	24.248	10.431	-0.942	1.00 38.47
ATOM	1826	0	LEU	1672	23.958	11.625	-0.898	1.00 42.25
MOTA	1827	N	PHE	1673	24.924	9.901	-1.956	1.00 39.07
ATOM	1829	CA	PHE	1673	25.414	10.725	-3.053	1.00 38.00
ATOM	1830	CB	PHE	1673	26.699	10.110	-3.639	1.00 36.48
ATOM	1831	CG	PHE	1673	27.826	9.928	-2.637	1.00 33.36
ATOM	1832		PHE	1673	28.524	8.724	-2.580	1.00 29.55
ATOM	1833	CD2		1673	28.205	10.960	-1.779	1.00 31.85
ATOM	1834	CE1		1673	29.580	8.540	-1.692	1.00 26.33
ATOM	1835		PHE	1673	29.265	10.786	-0.880	1.00 30.95
ATOM	1836	CZ	PHE	1673	29.954	9.568	-0.838	1.00 28.99
MOTA	1837	C	PHE	1673	24.413	10.957	-4.194	1.00 39.64
ATOM	1838	0	PHE	1673	24.364	12.046	-4.760	1.00 37.72
ATOM	1839	N	ASP	1674	23.651	9.928	-4.554	1.00 41.35
ATOM	1841	CA	ASP	1674	22.716	10.027	-5.666	1.00 43.38
ATOM	1842	CB	ASP	1674	22.934	8.858	-6.625	1.00 47.84
ATOM	1843	CG	ASP	1674	24.359	8.765	-7.121	1.00 53.24

ATOM	1844	OD1	ASP	1674	25.049	9.808	-7.172	1.00 56.20
MOTA	1845	OD2	ASP	1674	24.786	7.640	-7.460	1.00 55.73
ATOM	1846	C	ASP	1674	21.239	10.083	-5.321	1.00 45.94
ATOM	1847	0	ASP	1674	20.402	10.200	-6.222	1.00 47.80
ATOM	1848	N	ARG	1675	20.903	9.953	-4.040	1.00 45.98
ATOM	1850	CA	ARG	1675	19.503	9.981	-3.608	1.00 43.76
MOTA	1851	CB	ARG	1675	18.872	11.346	-3.887	1.00 48.61
MOTA	1852	CG	ARG	1675	19.519	12.478	-3.142	1.00 58.37
MOTA	1853	CD	ARG	1675	19.468	13.715	-3.992	1.00 70.39
MOTA	1854	NE	ARG	1675	20.035	14.867	-3.306	1.00 79.14
MOTA	1856	CZ	ARG	1675	19.612	16.116	-3.472	1.00 82.95
ATOM	1857	NH1	ARG.	1675	18.610	16.386	-4.308	1.00 82.00
ATOM	1860	NH2	ARG	1675	20.194	17.097	-2.793	1.00 87.42
MOTA	1863	С	ARG	1675	18.647	8.882	-4.236	1.00 39.26
ATOM	1864	0	ARG	1675	17.461	9.074	-4.488	1.00 37.29
ATOM	1865	N	ILE	1676	19.270	7.746	-4.526	1.00 35.86
MOTA	1867	CA	ILE	1676	18.544	6.614	-5.081	1.00 32.76
MOTA	1868	CB	ILE	1676	19.324	5.927	-6.192	1.00 31.73
ATOM	1869	CG2	ILE	1676	18.450	4.902	6.868	1.00 30.02
MOTA	1870	CG1	ILE	1676	19.767	6.955	-7.219	1.00 32.68
MOTA	1871	CD1	ILE	1676	20.658	6.371	-8.272	1.00 35.75
MOTA	1872	С	ILE	1676	18.329	5.625	-3.946	1.00 31.08
MOTA	1873	0	ILE	1676	19.264	4.962	-3.505	1.00 28.77
MOTA	1874	N	TYR	1677	17.102	5.558	-3.444	1.00 30.32
ATOM	1876	CA	TYR	1677	16.779.	4.653	-2.348	1.00 29.68
ATOM	1877	CB	TYR	1677	15.846	5.329	-1 354	1.00 31.14
ATOM	1878	CG	TYR	1677	16.523	6.395	-0.514	1 00 32.95
ATOM	1879	CD1		1677	16.616	7.721	-0.958	1.00 30.40
MOTA	1880	CE1		1677	17.208	8.707	-0.171	1.00 27.57
MOTA	1881		TYR	1677	17.048	6.082	0.743	1.00 32.13
ATOM	1882		TYR	1677	17.642	7.059	1.543	1.00 31.50
ATOM	1883	CZ	TYR	1677	17.711	8.366	1.081	1.00 31.12
MOTA	1884	OH	TYR	1677	18.235	9.326	1.912	1.00 32.18
ATOM	1886	C	TYR	1677	16.123	3.424	-2.933	1.00 28.88
ATOM	1887	0	TYR	1677	15.268	3.537	-3.811	1.00 32.20
ATOM	1888	N	THR	1678	16.556	2.253	-2.481	1.00 26.34
MOTA	1890	CA	THR	1678	16.023	0.988	-2.971	1.00 25.55
MOTA	1891	CB	THR	1678	16.917	0.394	-4.043	1.00 28.81
ATOM	1892	OG1	THR	1678	18.221	0.179	-3.483	1.00 34.06
ATOM	1894	CG2		1678	17.010	1.320	-5.267	1.00 27.25
ATOM	1895	C	THR	1678	16.037	0.007	-1.827	1.00 21.78
ATOM	1896	0	THR	1678	16.505	0.312	-0.744	1.00 25.57
MOTA	1897	N	HIS	1679	15.559	~1.198	-2.071	1.00 20.86
MOTA	1899	CA	HIS	1679	15.580	-2.216	-1.030	1.00 20.30
MOTA	1900	CB	HIS	1679	14.816	-3.453	-1.499	1.00 17.22
ATOM	1901	CG	HIS	1679	13.367	-3.196	-1.797	1.00 19.02
ATOM	1902	CD2		1679	12.662	-3.275	-2.958	1.00 14.89
MOTA	1903	ND1		1679	12.459	-2.830	-0.826	1.00 18.98
MOTA	1905	CE1		1679	11.260	-2.697	-1.370	1.00 16.10
MOTA	1906	NE2		1679	11.359	-2.961	-2.663	1.00 15.18
MOTA	1908	C	HIS	1679	17.050	-2.535	-0.761	1.00 20.44
ATOM	1909	0	HIS	1679	17.428	-2.901	0.356	1.00 22.58

-1.781 1.00 20.58 **MOTA** 1910 N GLN 1680 17.874 -2.310 1.00 22.70 1680 -1.721 **ATOM** 1912 CA GLN 19.303 -2.539 GLN 1680 19.935 -2.427 -3.106 1.00 26.26 **ATOM** 1913 CB **ATOM** GLN 1680 19.934 -3.711-3.889 1.00 31.86 1914 CG -3.687 -5.026 **ATOM** 1915 CD GLN 1680 18.949 1.00 37.54 MOTA 1916 OE1 GLN 1680 17.931 -3.000 -4.961 1.00 42.70 **ATOM** 1917 NE2 GLN 1680 19.256 -4.409 -6.091 1.00 37.42 -0.797 **ATOM** 1920 C GLN 1680 19.985 -1.559 1.00 24.93 **ATOM** 1921 O GLN 1680 20.875 -1.943 -0.039 1.00 26.39 **ATOM** 1922 N SER 1681 19.605 -0.286 -0.867 1.00 24.70 **ATOM** 1681 1924 CA SER 20.239 0.678 0.030 1.00 23.24 MOTA 1925 CB SER 1681 19.923 2.128 -0.346 1.00 19.33 MOTA 1926 OG SER 1681 18.544 2.326. -0..545. 1.00 18.55 **ATOM** 1928 C SER 1681 19.852 0.364 1.464 1.00 21.77 MOTA 1929 0.609 1.00 24.14 0 SER 1681 20.645 2.36€ MOTA 1930 ASP -0.210 1.670 N 1682 18.659 1.00 21.80 MOTA 1932 CA **ASP** 1682 18.180 -0.604 3.003 1.00 22.45 MOTA 1933 CB **ASP** 1682 16.730 -1.111 2.963 1.00 25.27 MOTA 1934 CG ASP 1682 15.678 0.004 3.132 1.00 28.21 MOTA 1935 OD1 ASP 1682 14.500 -0.245 2.786 1.00 25.41 MOTA 1936 OD2 ASP 1682 15.992 1.102 3.639 1.00 30.19 **ATOM** 1937 C ASP 1682 19.076 -1.736 3.517 1.00 23.69 ASP **ATOM** 1.00 24.74 1.938 O 1682 19.385 -1.799 4.709 **ATOM** 1939 N VAL 1683 19.474 -2.6352.620 1.00 23.49 **ATOM** 1941 CA VAL 1683 20.354 -3.7373.003 1.00 21.77 MOTA 1942 CB VAL 1683 -4.741 1.837 1.00 20.49 20.543 MOTA CG1 VAL ..5.613 1943 1683 21.770 2.039 1 00 19.82 **ATOM** 1944 CG2 VAL 1683 19.320 -5.618 1.736 1.00 19.29 **ATOM** 1945 C VAI. 1683 21.674 -3.153 3.523 1.00 21.93 **ATOM** 1946 0 VAL 1683 22.161 -3.570 4.573 1.00 21.06 ATOM 1947 N TRP 1684 22.207 -2.143 2.837 1.00 20.64 **ATOM** 1949 CA TRP 1684 23.424 -1.482 3.295 1.00 20.98 **ATOM** 1950 CB 16**B**4 -0.224 1.00 19.56 TRP 23.711 2.463 ATOM 1951 CG TRP 1684 24.859 0.609 2.970 1.00 23.22 **ATOM** 1952 CD2 TRP 1684 26.182 0.686 2.421 1.00 24.64 **ATOM** 1953 CE2 TRP 1684 1.559 1.00 24.69 26.929 3.249 **ATOM** CE3 TRP 1954 1684 0.102 1.315 1.00 26.41 26.813 **ATOM** 1955 CD1 TRP 1684 4.075 1.00 23.64 24.857 1.430 MOTA 1956 NE1 TRP 1684 1.994 1.00 23.28 26.097 4.246 **ATOM** 1958 CZ2 TRP 1684 28.275 1.859 3.000 1.00 20.55 ATOM 1959 CZ3 TRP 1684 28.165 0.409 1.072 1.00 22.82 MOTA 1960 CH2 TRP 1684 28.872 1.274 1.908 1.00 19.24 1961 **ATOM** C TRP 1684 23.201 -1.112 4.771 1.00 21.12 **ATOM** 1962 0 TRP 1684 23.931 -1.560 5.652 1.00 22.08 ATOM 1963 N SER 1685 22.150 -0.3425.032 1.00 23.27 **ATOM** 1965 CA SER 1685 21.787 0.086 6.386 1.00 22.54 **ATOM** 1966 CB SER 1685 20.429 0.768 6.356 1.00 21.98 **MOTA** 1967 OG SER 1685 1.626 20.318 5.220 1.00 25.48 **ATOM** 1969 C SER 7.389 1685 21.747 -1.068 1.00 21.33 **ATOM** 1.00 19.52 1970 0 SER 1685 22.145 -0.902 8.545 **ATOM** 1971 N PHE 1686 21.260 -2.22B 6.946 1.00 23.10 ATOM 1973 CA PHE 1686 21.174 -3.424 7.800 1.00 23.09

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ATOM	1974	CB	PHE	1686	20.409	-4.550	7.095	1.00 22.77
ATOM	1975	CG	PHE	1686	20.192	-5.767	7.962	1.00 25.82
ATOM	1976	CD	L PHE	1686	19.378	-5.694	9.096	1.00 25.54
MOTA	1977	CD2	2 PHE	1686	20.808	-6.987	7.649	1.00 23.88
MOTA	1978	CE	PHE	1686	19.185	-6.809	9.913	1.00 24.25
MOTA	1979	CE2	PHE	1686	20.622	-8.109	8.455	1.00 22.67
MOTA	1980	CZ	PHE	1686	19.809	-8.023	9.585	1.00 26.30
ATOM	1981	C	PHE	1686	22.569	-3.919	8.240	1.00 21.77
ATOM	1982	0	PHE	1686	22.739	-4.450	9.350	1.00 20.47
MOTA	1983	N	GLY	1687	23.553	-3.773	7.358	1.00 20.63
ATOM	1985	CA	GLY	1687	24.913	~4.163	7.685	1.00 19.29
ATOM	1986	C	GLY	1687	25.407 ·	-3.276	8.822	1.00 21.64
MOTA	1987	~ O	GLY	1687	26.094	-3.755	9.727	1:00 19:46
MOTA	1988	N	LAV	1688	25.008	-1.996	8.794	1.00 22.19
MOTA	1990	CA	VAL	1688	25.372	-1.024	9.831	1.00 21.99
ATOM	1991	CB	VAL	1688	25.048	0.458	9.423	1.00 23.20
ATOM	1992	CG1	VAL	1688	25.439	1.424	10.540	1.00 21.22
ATOM	1993	CG2	VAL	1688	25.820	0.846	8.161	1.00 21.25
ATOM	1994	C	VAL	1688	24.621	-1.403	11.100	1.00 23.33
ATOM	1995	Ó	VAL	1688	25.204	-1.420	12.187	1.00 24 98
ATOM	1996	N	LEU	1689	23.339	-1.734	10.969	1.00 24.36
MOTA	1998	CA	LEU	1689	22.542	-2.161	12.122	1.00 23.92
MOTA	1999	CB	LEU	1689	21.072	-2.392	11.714	1.00 22.57
ATOM	2000	CG	LEU	1689	19.981	-2.427	12.805	1.00 23.41
MOTA	2001		I.EU	1689	18.614	-2.295	12.164	1.30 19.14
MOTA	2002	CD2		1689	20.048	-3.700	13.658	1.00 22.75
ATOM	2003	С	LEU	1689	23.158	-3.447	12.717	1.00 25.22
ATOM	2004	C	LEU	1689	23.202	-3.592	13.937	1.00 25.58
ATOM	2005	N	LEU	1690	23.514	-4.379	11.871	1.00 25.47
ATOM	2007	CA	LEU	1690	24.256	-5.604	12.376	1.00 26.26
ATOM	2008	CB	LEU	1690	24.730	-6.531	11.255	1.00 26.22
ATOM	3009	CG	LEU	1690	23.809	-7.501	10.515	1.00 26.21
ATOM	2010		LEU	1690	24.662	-8.259	9.523	1.00 25.45
ATOM ATOM	2011		LEU	1690	23.135	-8.487	11.458	1.00 21.17
ATOM	2012	C	LEU	1690	25:471	-5.204	13.189	1.00 26.51
ATOM	2013	0	LEU	1690	25.710	-5.747	14.273	1.00 29.07
ATOM	2014	N	TRP	1691	26.240	-4.255	12.660	1.00 26.26
ATOM	2016 2017	CA	TRP	1691	27.431	-3.761	13.341	1.00 25.08
ATOM	2017	CB CG	TRP	1691	28.129	-2.706	12.493	1.00 25.16
ATOM	2019		TRP	1691	29.456	-2.268	13.039	1.00 27.49
ATOM	2020	CE2	TRP	1691	29.701	-1.163	13.925	1.00 25.81
ATOM	2021	CE3		1691	31.100	-1.070	14.103	1.00 22.63
ATOM	2022			1691	28.870	-0.236	14.575	1.00 26.70
ATOM	2023	CD1	TRP	1691	30.688	-2.798	12.735	1.00 23.03
ATOM	2025	NE1	TRP	1691	31.675	-2.078	13.371	1.00 25.19
ATOM	2025	CZ2	TRP	1691	31.690	-0.085	14.900	1.00 18.66
ATOM	2026	CZ3 CH2	TRP	1691	29.459	0.745	15.371	1.00 25.66
ATOM	2027	CHZ		1691	30.861	0.812	15.523	1.00 23.00
ATOM	2029	0	TRP TRP	1691	27.114	-3.195	14.727	1.00 24.63
ATOM	2030	N	GLU	1691	27.871	-3.393	15.662	1.00 27.79
ATOM	2030	CA		1692	25.985	-2.506	14.862	1.00 26.48
•••	2032	CH	GLU	1692	25.574	-1.938	16.155	1.00 24.98

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-1.060 MOTA 2033 GLU CB 1692 24.335 15.994 1.00 22.29 MOTA 2034 CG GLU 1692 24.507 0.107 15.056 1.00 18.31 **ATOM** 2035 CD GLU 1692 23.255 0.933 14.978 1.00 25.10 ATOM 2036 OE1 GLU 1692 22 433 0.704 14.066 1.00 26.95 2037 **ATOM** OE2 GLU 1692 23.067 1.815 15.840 1.00 27.05 **ATOM** 2038 C GLU 1692 25.260 -3.036 17.163 1.00 25.18 ATOM 2039 0 GLU 1692 25.602 -2.927 18.341 1.00 26.12 **ATOM** 2040 N ILE 1693 -4.087 16.698 24.593 1.00 27.16 **ATOM** 2042 CA ILE 1693 24.231 -5.214 17.555 1.00 25.91 **ATOM** 2043 CB ILE 1693 23.373 -6.287 16.777 1.00 25.70 ATOM 2044 CG2 ILE 23.171 1693 -7.564 17.638 1.00 18.73 MOTA 2045 CG1 ILE 1693 22.005 -5.682 16.382 1.00 23.45 MOTA 2046 CD1. ILE 1693 21.208 -6.485 15.346 1.00 15.62 **ATOM** 2047 1.00 26.70 C ILE 1693 25.496 -5.847 18.107 **ATOM** 2048 0 ILE 1693 25.672 -5.961 19.316 1.00 28.19 **ATOM** 2049 N PHE 1694 26.442 -6.133 17.229 1.00 28.78 ATOM 2051 CA PHE 1694 27.664 -6.779 17.679 1.00 29.72 ATOM 2052 CB PHE 1694 28.261 -7.598 16.542 1.00 27.18 ATOM 2053 CG PHE 1694 27.315 -8.649 16.048 1.00 25.38 **ATOM** 2054 CDl PHE 1694 26.793 -8.599 14.770 1.00 26.16 **ATOM** 2055 CD2 PHE 1694 26.844 -9.625 16.919 1.00 26.37 ATOM 2056 CE1 PHE 1694 25.808 -9.505 14.370 1.00 31.37 **ATOM** 2057 PHE CE2 1694 25.863 -10.533 16.536 1.00 25.23 **ATOM** 2058 CZPHE .1694 25.337 -10.478 15.268 1.00 29.46 MOTA 2059 PHE C 1694 28.663 -5.906 18.438 1.00 30.92 ATOM 2060 C PHE 1694 29.697 -6.403 18.902 1.00 32.23 **ATOM** 5061 N THR 1695 28.344 -4.616 18.575 1.00 29 46. ATOM 2063 CA THR 1695 29.170 -3.698 19.348 1.00 27.17 **ATOM** 2064 CB THR 1695 29.665 -2.474 18.535 1.00 23.32 **ATOM** -1.710 2065 OG1 THR 1695 28.553 18.046 1.00 24.73 MOTA 2067 CG2 THR 1695 -2.914 30.538 17.395 1.00 21.34 **ATOM** 2068 C THR 1695 28.307 -3.230 20.519 1.00 28.81 MOTA 2069 0 THR 1695 28.707 -2.34621,289 1.00 31.85 ATOM 2070 N LEU 1696 27.130 -3.841 20.651 1.00 26.30 ATOM 2072 CA LEU 1696 26.188 -3.523 21,720 1.00 25.99 MOTA 2073 CB LEU 1696 26.704 -4.043 23.060 1.00 24.51 **ATOM** 2074 CG LEU 1696 26.974 -5.539 23.194 1.00 23.32 MOTA 2075 CD1 LEU 1696 27.447 -5.843 24.597 1.00 26.45 **ATOM** 2076 CD2 LEU 1696 25.726 -6.297 22.907 1.00 29.79 ATOM 2077 C LEU 1696 25.892 -2.036 21.837 1.00 24.90 MOTA 2078 0 LEU 1696 26.083 -1.457 22.889 1.00 28.99 **ATOM** 2079 N GLY 1697 25.386 -1.432 20.771 1.00 25.05 MOTA 2081 CA GLY 1697 25.072 -0.016 20.811 1.00 24.31 **ATOM** 2082 С GLY 1697 26.241 0.847 20.381 1.00 27.15 MOTA 2083 GLY 26.297 0 1697 2.035 20.701 1.00 29.57 MOTA 2084 GLY N 1698 27.177 0.261 19.639 1.00 27.33 **ATOM** 2086 CA GLY 1698 28.319 1.023 19.178 1.00 27.04 ATOM 2087 C GLY 1698 27.966 2.109 18.173 1.00 29.78 ATOM 2088 0 GLY 1698 27.115 1.929 17.301 1.00 32.03 ATOM 2089 N SER 1699 28.633 3.247 18.295 1.00 30.60 ATOM 2091 CA SER 1699 28.413 4.385 17.414 1.00 31.48 ATOM 2092 CB SER 1699 28.747 5.692 18.164 1.00 32.97

ATOM	2093	OG	SER	1699	28.350	6.848	17.436	1.00 37.75
ATOM	2095	C	SER	1699	29.323	4.239	16.188	1.00 32.74
ATOM	2096	0	SER	1699	30.541	4.034	16.321	1.00 33.04
MOTA	2097	N	PRO	1700 .	28.732	4.276	14.979	1.00 31.40
MOTA	2098	CD	PRO	1700	27.288	4.320	14.688	1.00 30.88
MOTA	2099	CA	PRO	1700	29.507	4.153	13.737	1.00 30.55
MOTA	2100	CB	PRO	1700	28.420	4.024	12.657	1.00 30.13
ATOM	2101	CG	PRO	1700	27.228	3.535	13.398	1.00 31.10
ATOM	2102	С	PRO	1700	30.300	5.427	13.509	1.00 31.19
MOTA	2103	0	PRO	1700	29.766	6.522	13.651	1.00 35.48
ATOM	2104	N	TYR	1701	31.574	5.277	13.175	1.00 29.51
ATOM	2106	CA	TYR	1701	32.446	6.412	12.899	1.00 30.10
ATOM	2107	CB	TYR	1701	32.084	7.029	11.541	1.00 32.84
ATOM	2108	CG	TYR	1701	32.102	6.078	10.353	1.00 38.43
ATOM	2109	CD1	TYR	1701	30.921	5.795	9.643	1.00 40.14
ATOM	2110	CEl	TYR	1701	30.930	5.000	8.513	1.00 39.07
ATOM	2111	CD2	TYR	1701	33.298	5.522	9.890	1.00 38.19
ATOM	2112	CE2	TYR	1701	33.320	4.726	8.754	1.00 41.52
ATOM	2113	CZ	TYR	1701	32.134	4.471	8.067	1.00 44.97
ATOM	2114	ОН	TYR	1701	32.151	3.700	6.919	1.00 54.77
ATOM	2116	С	TYR	1701	32.426	7.524	13.965	1.00 30.38
ATOM	2117	0	TYR	1701	32.009	8.655	13.685	1.00 30.54
ATOM	2118	N	PRO	1702	32.947	7.239	15.170	1.00 30.61
MOTA	2119	CD	PRO	1702	33.578	5.985	15.608	1.00 29.72
ATOM	2120	CA	PRO	1702	32.971	8.239	16.248	1.00 28.48
ATOM	2121	CB	PRO	1702	33.554	7.463	17.429	1.00 28.43
ATOM	2122	CG	PRO	1702	33.320	6.025	17.085	1.00 30.63
ATOM	2123	C	PRO	1702	33.897	9.385	15.981	1.00 26.93
MOTA	2124	0	PRO	1702	34.998	9.156	15.418	1 00 26.21
ATOM	2125	N	GLY	1703	33.440	10.613	16.084	1.00 29.51
ATOM	2127	CA	GLY	1703	34.239	11.787	15.767	1.00 28.57
ATOM	2128	С	GLY	1703	34.374	12.143	14.296	1.00 28.97
ATOM	2129	0	GLY	1703	35.055	13.104	13.962	1.00 29.54
ATOM	2130	N	VAL	1704	33.726	11.380	13.418	1.00 30.90
ATOM	2132	CA	VAL	1704	33.798	11.616	11.975	1.00 29.48
ATOM	2133	CB	VAL	1704	33.806	10.289	11.228	1.00 28.23
MOTA	2134	CG1	VAL	1704	34.074	10.525	9.750	1.00 31.57
MOTA	2135	CG2	VAL	1704	34.851	9.375	11.822	1.00 28.40
ATOM	2136	C	VAL	1704	32.620	12.466	11.477	1.00 33.14
ATOM	2137	0	VAL	1704	31.466	12.045	11.529	1.00 35.67
ATOM	2138	N	PRO	1705	32.906	13.681	10.979	1.00 35.22
ATOM	2139	CD	PRO	1705	34.217	14.348	11.008	1.00 38.03
ATOM	2140	CA	PRO	1705	31.868	14.587	10.474	1.00 35.96
ATOM	2141	CB	PRO	1705	32.534	15.953	10.627	1.00 35.84
MOTA	2142	CG	PRO	1705	33.939	15.661	10.279	1.00 37.29
ATOM	2143	С	PRO	1705	31.473	14.293	9.031	1.00 37.17
MOTA	2144	0	PRO	1705	32.255	13.690	8.288	1.00 38.39
ATOM	2145	N	VAL	1706	30.296	14.780	8.624	1.00 36.10
ATOM	2147	CA	VAL	1706	29.743	14.582	7.276	1.00 37.10
ATOM	2148	СВ	VAL	1706	28.667	15.658	6.942	1.00 38.36
MOTA	2149	CG1	VAL	1706	28.106	15.441	5.535	1.00 38.93
MOTA	2150	CG2	VAL	1706	27.536	15.595	7.952	1.00 40.79

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14.559 **ATOM** 2151 С VAL 1706 30.762 6.138 1.00 37.09 ATOM 2152 13.543 0 VAL 1706 30.927 5.461 1.00 38.75 **ATOM** 2153 N **GLU** 1707 31.477 15.663 5.967 1.00 37.08 **ATOM** 2155 CA GLU 1707 32.472 15.793 4.910 1.00 35.52 **ATOM** CB 17.206 4.918 2156 GLU 1707 33.059 1.00 38.30 MOTA 2157 C GLU 1707 33.588 14.762 4.945 1.00 34.20 ATOM 2158 0 GLU 1707 34.153 14.445 3.908 1.00 33.48 **ATOM** 2159 1708 33.936 14.273 N GLU 6.132 1.00 34.20 ATOM 2161 CA GLU 1708 34.981 13.256 6.241 1.00 36.08 MOTA 2162 CB GLU 1708 35.555 13.178 7.660 1.00 40.39 **ATOM** 2163 CG GLU 1708 36.212 14.464 8.179 1.00 45.41 MOTA 2164 CD GLU 1708 37.471 14.871 7.430 1.00 50.66 **ATOM** 2165 OE1 GLU 1708 38.199 13.986 6.909 1.00 54.73 **ATOM** 16.092 2166 OE2 GLU 1708 37.747 7.392 1.00 52.85 **ATOM** 2167 C GLU 1708 34.369 11.911 5.855 1.00 35.22 **ATOM** 2168 0 GLU 1708 35.035 11.045 5.260 1.00 34.04 ATOM 2169 N LEU 1709 33.0B9 11.745 6.178 1.00 33.30 MOTA 2171 CA LEU 1709 32.376 10.519 5.860 1.00 31.44 MOTA 2172 CB LEU 1709 30.975 10.531 6.474 1.00 26.89 MOTA 2173 CG LEU 1709 30.065 9.365 6.073 1.00 26.05 LEU MOTA 2174 8.036 CD1 1709 30.652 6.503 1.00 22.75 ATOM 2175 CD2 LEU 1709 28.717 9.574 6.537 1.00 26.15 ATOM 2176 C LEU 32.291 10.325 1709 4.350 1.00 31.18 ATOM 9.209 LEU 2177 0 1709 32.490 3.856 1.00 29.88 ATOM 2178 N PHE 32.011 11.408 1710 3.623 1.00 30.16 **ATOM** 2180 CA PHE 1710 31.915 11.333 2.169 1.00 31.64 **ATOM** 2181 CB PHE 1710 31.658 12.710 1.567 1.00 33.44 **ATOM** 2182 CG PHE 1710 30.287 13.231 1.827 1.00 37.78 CD1 MOTA 2183 PHE 29.287 12.395 1710 2.303 1.00 41.46 **ATOM** 2184 CD2 PHE 1710 29.991 14.565 1.513 1.00 40.72 **ATOM** 2185 28.012 CEI PHE 1710 12.882 2.566 1.00 41.30 **ATOM** 28.715 2186 CE2 PHE 1710 15.058 1.875 1.00 42.99 **ATOM** 27.725 2187 CZ PHE 1710 14.208 2.354 1.00 40.95 **MOTA** 2188 C PHE 1710 33.202 10.771 1.609 1.00 32.38 MOTA 2189 O PHE 1710 33.183 9.815 0.825 1.00 32.26 **ATOM** 2190 LYS 34.310 11.336 2.085 N 1711 1.00 31.26 MOTA 2192 CA LYS 1711 35.664 10.971 1.697 1.00 29.73 MOTA 2193 CB LYS 1711 36.642 11.932 2.379 1.00 33.49 11.716 MOTA 2194 CG LYS 38.103 1711 2.042 1.00 39.79 MOTA 2195 LYS 38.981 CD 1711 12.731 2.755 1.00 43.35 **MOTA** 2196 40.413 CE LYS 1711 12.6B6 2.238 1.00 4€.23 **ATOM** 2197 NZ LYS 1711 41.116 11.422 2.600 1.00 53.67 **ATOM** 2201 LYS 1711 35.999 9.501 C 2.015 1.00 29.34 **ATOM** 2202 0 LYS 1711 36.670 8.836 1.231 1.00 28.77 **ATOM** 2203 LEU 1712 35.541 9.000 N 3.164 1.00 30.40 ATOM 2205 CA LEU 1712 35.776 7.599 3.532 1.00 28.72 **ATOM** 2206 LEU 35.241 CB 1712 7.295 4.942 1.00 27.71 ATOM 2207 CG LEU 1712 35.971 7.870 6.166 1.00 28.23 ATOM 2208 CD1 LEU 1712 35.186 7.593 7.440 1.00 20.80 ATOM 2209 CD2 LEU 1712 37.389 7.297 6.266 1.00 27.01 MOTA 35.022 2210 C LEU 1712 6.738 2.530 1.00 30.03 **ATOM** LEU 35.571 5.796 2211 0 1712 1.957 1.00 29.28

MOTA	2212	N	LEU	1713	33.752	7.073	2.325	1.00 31.98
ATOM	2214	CA	LEU	1713	32.904	6.339	1.403	1.00 34.30
ATOM	2215	CB	LEU	1713	31.467	6.872	1.447	1.00 37.65
MOTA	2216	CG	LEU	1713	30.663	6.450	2.686	1.00 37.06
MOTA	2217	CD1	LEU	1713	29.367	7.217	2.781	1.00 36.80
ATOM	2218	CD2	LEU	1713	30.399	4.950	2.641	1.00 37.02
ATOM	2219	С	LEU	1713	33.451	6.344	-0.011	1.00 35.45
ATOM	2220	0	LEU	1713	33.468	5.298	-0.662	1.00 38.18
ATOM	2221	N	LYS	1714	33.920	7.498	-0.481	1.00 33.22
ATOM	2223	CA	LYS	1714	34.487	7.590	-1.821	1.00 31.46
ATOM	2224	СВ	LYS	1714	34.881	9.027	-2.158	1.00 31.32
ATOM	2225	CG	LYS	1714	33.724	9.962	-2.399	1.00 33.49
ATOM -	2226	CD	LYS	1714	32.814		-3.491	1.00 39.40
ATOM	2227	CE	LYS	1714	31.613	10.364	-3.720	1.00 44.79
ATOM	2228	NZ	LYS	1714	30.674	9.841	-4.771	1.00 50.41
ATOM	2232	С	LYS	1714	35.706	6.678	-1.953	1.00 32.53
ATOM	2233	0	LYS	1714	35.998	6.155	-3.025	1.00 35.46
ATOM	2234	N	GLU	1715	36.420	6.488	-0.856	1.00 33.50
ATOM	2236	CA	GLU	1715	37.602	5.644	-0.864	1.00 33.30
ATOM	2237	СВ	GLU	1715	38.617	5.177	0.143	1.00 37.20
ATOM	2238	CG	GLU	1715	39.085	7.571	-0.221	1.00 37.20
ATOM	2239	CD	GLU	1715	39.654	8.372	0.946	1.00 51.44
ATOM	2240	OE1		1715	39.820	7.826	2.065	1.00 51.40
ATOM	2241	OE2	GLU	1715 .	39.930	9.573	0.726	1.00 54.23
ATOM	2242	c	GLU	1715	37.278	4.183	-0.581	1.00 35.09
ATOM	2243	0	GLU	1715	38.184	3.357	-0.482	1.00 37.59
ATOM	2244	N	GLY	1716	35.991	3.866	-0.455	1.00 37.39
ATOM	2246	CA	GLY	1716	35.576	2.498	-0.197	1.00 30.96
ATOM	2247	С	GLY	1716	35.852	1.976	1.198	1.00 29.06
ATOM	2248	0	GLY	1716	35.906	0.766	1.416	1.00 29.28
ATOM	2249	N	HIS	1717	35.995	2.8.79	2.155	1.00 28.16
ATOM	2251	CA	HIS	1717	36.282	2.489	3.532	1.00 29.80
ATOM	2252	СВ	HIS	1717	36.534	3.743	4.378	1.00 33.13
ATOM	2253	CG	HIS	1717	36.794	3.469	5.826	1.00 36.22
ATOM	2254	CD2		1717	37.955	3.375	6.516	1.00 35.38
ATOM	2255	ND1		1717	35.782	3.279	6.746	1.00 37.81
MOTA	2257	CE1	HIS	1717	36.309	3.080	7.942	1.00 36.97
ATOM	2258	NE2		1717	37.624	3.134	7.830	1.00 35.83
ATOM	2260	С	HIS	1717	35.171	1.645	4.153	1.00 29.26
ATOM	2261	0	HIS	1717	33.987	1.900	3.940	1.00 31.43
ATOM	2262	N	ARG	1718	35.571	0.666	4.955	1.00 28.11
ATOM	2264	CA	ARG	1718	34.632	-0.212	5.640	1.00 30.67
ATOM	2265	СВ	ARG	1718	34.592	-1.583	4.973	1.00 27.32
ATOM	2266	CG	ARG	1718	34.058	-1.586	3.557	1.00 28.77
ATOM	2267	CD	ARG	1718	32.609	-1.111	3.484	1.00 28.84
ATOM	2268	NE	ARG	1718	32.032	-1.167	2.131	1.00 24.96
ATOM	2270	CZ	ARG	1718	32.141	-0.206	1.204	1.00 24.90
ATOM	2271	NH1		1718	32.824	0.912	1.454	1.00 20.04
ATOM	2274	NH2		1718	31.513	-0.338	0.045	1.00 20.04
ATOM	2277	C	ARG	1718	35.091	-0.350	7.101	1.00 20.04
ATOM	2278	Ö	ARG	1718	36.300	-0.449	7.377	1.00 36.48
ATOM	2279	N	MET	1719	34.134	-0.355	8.028	1.00 36.48
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	ATOM	2281	CA	MET	1719	34.428	-0.459	9.448	1.00 32.33
	ATOM	2282	CB	MET	1719	33.148	-0.285	10.277	1.00 34.72
	ATOM	2283	CG	MET	1719	32.454	1.066	10.076	1.00 35.04
	MOTA	2284	SD	MET	1719	31.025	1.447	11.141	1.00 34.06
	ATOM	2285	CE	MET	1719	29.757	0.470	10.409	1.00 33.14
	ATOM	2286	С	MET	1719	35.068	-1.797	9.747	1.00 35.53
	ATOM.	2287	0	MET	1719	34.896	-2.756	8.991	1.00 35.48
	MOTA	2288	N	ASP	1720	35.826	-1.843	10.840	1.00 38.65
	ATOM	2290	CA	ASP	1720	36.521	-3.049	11.281	1.00 39.03
	ATOM	2291	CB	ASP	1720	37.659	-2.678	12.237	1.00 43.11
	MOTA	2292	CG	ASP	1720	38.743	-1.846	11.569	1.00 46.69
	ATOM	2293	OD1	ASP	1720	38:587	-1.536	10.364	1.00 54.08
	ATOM .	.2294	OD2	ASP	1720	39.750	-1.503	12.239	. 1.00 45.93
	MOTA	2295	C	ASP	1720	35.580	-4.023	11.972	1.00 38.50
	ATOM	2296	0	ASP	1720	34.554	-3.617	12.528	1.00 37.73
	MOTA	2297	N	LYS	1721	35.961	~5.298	11.981	1.00 38.10
	MOTA	2299	CA	LYS	1721	35.151	-6.339	12.600	1.00 38.12
	MOTA	2300	CB	LYS	1721	35.727	-7.733	12.323	1.00 38.20
	ATOM	2301	CG	LYS	1721	34.825	-8.858	12.825	1 00 38.48
	ATOM	2302	CD	LYS	1721	35.375	-19.238	12.543	1.00 37.49
	MOTA	2303	CE	LYS	1721	36.320	-1.0.691	13.625	1.00 39 11
	MOTA	2304	NZ	LYS	1721	36.448	-12.167	13.628	1.00 40.75
	ATOM	2308	С	LYS	1721	35.092	-6.142	14.091	1.00 40.24
	ATOM	2309	0	LYS	1721	36.136	-6.032	14 739	1.70 42.70
	MOTA	2310	N	PRO	1722	33.875	-6.082	14.658	1.00 41.23
	ATOM	2311	CD	PRO	1722	32.547	-6.153	14.019	1.00 38.63
	ATOM	2312	CA	PRO	1722	33.743	-5.901	16.104	1.00 41.71
	ATOM	2313	CB	PRO	1722	32.223	-5.957	16.306	1.00 38.90
	ATOM	2314	CG	PRO	1722	31.679	-5.442	15.016	1.00 34.19
	ATOM	2315	c	PRO	1722	34.418	-7.079	16.819	1.00 43.96
	ATOM	2316	0	PRO	1722	34.542	-8.174	16.250	1.00 43.02
	MOTA	2317	N	SER	1723	34.915	-6.860	18.028	1.00 46.76
	MOTA	2319	CA	SER	1723	35.493	-7.973	18.747	1.00 50.74
	ATOM	2320	CB	SER	1723	36.265	-7.500	19.980	1.00 49.47
	ATOM	2321	OG	SER	1723	35.400	-7.130	21.035	1.00 53.87
	MOTA	2323	C	SER	1723	34.259	-8.782	19.143	1.00 53.24
	ATOM	2324	0	SER	1723	33.136	-8.259	19.130	1.00 53.97
	ATOM	2325	N	ASN	1724		-10.064	19.426	1.00 56.59
	ATOM	2327	CA	ASN	1724		-10.899	19.825	1.00 59.55
	ATOM ATOM	2328 2329	CB	ASN	1724 1724		-10.386	21.162	1.00 66.12
	ATOM ATOM	2329	CG OD1	ASN	1724		-10.128	22.213	1.00 71.34
	ATOM	2331	ND2				-10.990	22.485	1.00 73.38
	ATOM	2334	C	ASN	1724		-8.926	22.779	1.00 74.19
	ATOM				1724		-10.900	18.711	1.00 57.31
	ATOM ATOM	2335 2336		ASN CYS	1724		-10.662	18.940	1.00 59.27
			N		1725		-11.132	17.493	1.00 54.50
	ATOM	2338	CA	CYS	1725		-11.203	16.300	1.00 50.89
	ATOM ATOM	2339	CB	CYS	1725			15.576	1.00 50.09
	ATOM ATOM	2340	SG	CYS	1725	30.893	-9.833	14.006	1.00 44.81
	ATOM	2341	C	CYS	1725			15.439	1.00 47.28
	ATOM	2342	0	CYS	1725		-12.172	15.288	1.00 48.97
•	ATOM	2343	N	THR	1726	21.863	-13.229	14.950	1.00 42.60

ATOM	2345	CA	THR	1726	32.472	-14.275	14.139	1.00 39.22
ATOM	2346	CB	THR	1726	31.520	-15.494	13.984	1.00 36.36
MOTA	2347	OG1	THR	1726	30.290	-15.087	13.363	1.00 36.62
MOTA	2349	CG2	THR	1726	31.210	-16.084	15.326	1.00 33.12
ATOM	2350	С	THR	1726	32.858	-13.748	12.776	1.00 37.99
MOTA	2351	ο.	THR	1726	32.373	-12.704	12.357	1.00 39.57
MOTA	2352	N	ASN	1727	33.724	-14.473	12.080	1.00 37.02
ATOM	2354	CA	ASN	1727	34.133	-14.044	10.742	1.00 38.17
ATOM	2355	CB	ASN	1727	.35.290	-14.880	10.221	1.00 40.63
ATOM	2356	CG	ASN	1727	36.580	-14.593	10.953	1.00 44.79
ATOM	2357	OD1	ASN	1727	37.188	-13.539	10.781	1.00 46.57
ATOM	2358	ND2	ASN	1727	37.010	-15.536	11.778	1.00 48.30
ATOM	2361	C	ASN	1727	32.958	-14.159	9.786	1.00 38.22
ATOM	2362	0	ASN	1727	32.883	-13.431	8.793	1.00 39.53
ATOM	2363	N	GLU	1728	32.041	15.076	10.093	1.00 37.33
MOTA	2365	CA	GLU	1728	30.854	-15.312	9.273	1.00 34.24
ATOM	2366	CB	GLU	1728	30.109	-16.551	9.765	1.00 32.82
MOTA	2367	CG	GLU	1728	28.973	-17.000	8.855	1.00 35.84
ATOM	2368	CD	GLU	1.728	28.329	-18.306	9.297	1.00 42.16
MOTA	2369	OE1	GLU	1728	28.409	-18.633	LO.504	1.00 46.78
ATOM	2370	OE2	GLU	5.728	27.734	-18.996	8.440	1.00 38.81
ATOM	2371	C	GLU	1728	29.925	-14.104	9.313	1.00 33.05
ATOM	2372	0	GLU	1728	29.521	-13.574	8.272	1.00 25.58
ATOM	2373	N	LEU	1.729	29.608	-13.671	10.527	1.00 32.09
ATOM	2375	CA	LEU	1729	28.741	-12.530	10.710	1.90 32.45
ATOM	2376	СВ	TEA	1729	28.351	12.389	12.179	1.00 32.64
MOTA	2377	CG	LEU	1729	27.311	-13.431	12.575	1.00 34.65
MOTA	2378	CD1	LEU	1729	27.131	-13.388	i4.089	1.00 37.18
MOTA	2379	CD3	LEU	1729	25.988	-13.16?	11.842	1.00 27.77
ATOM	2380	C	LEU	1729	29.359	-11.252	10.175	1.00 32.68
ATOM	2381	0	LEU	1729	28.638	-10.367	9.693	1.00 31.97
MOTA	2382	N	TYR	1730	30.688	-11.143	10.251	1.00 31.70
MOTA	2384	C'A	TYR	1730	31.378	-9.959	9.734	1.00 30.19
MOTA	2385	CB	TYR	1730	32.849	-9.940	10.154	1.00 27.88
MOTA	2386	CG	TYR	1730	33.591	-8.723	9.649	1.00 26.63
MOTA	2387	CD1	TYR	1730	33.093	-7.449	9.879	1.00 27.37
MOTA	2388	CE1		1730	33.725	-6.324	9.378	1.00 27.56
MOTA	2389	CD2	TYR	1730	34.759	-8.849	8.904	1.00 24.07
ATOM	2390	CE2	TYR	1730	35.408	-7.724	8.393	1.00 24.81
MOTA	2391	CZ	TYR	1730	34.882	-6.462	8.631	1.00 28.56
MOTA	2392	OH	TYR	1730	35.473	-5.316	8.111	1.00 29.08
ATOM	2394	С	TYR	1730	31.287	-9.962	8.208	1.00 29.50
ATOM	2395	0	TYR	1730	31.062	-8.928	7.585	1.00 29.16
ATOM	2396	N	MET	1731	31.443	-11.139	7.623	1.00 31.05
ATOM	2398	CA	MET	1731		-11.313	6.187	1.00 34.59
ATOM	2399	CB	MET	1731		-12.779	5.840	1.00 41.42
MOTA	2400	CG	MET	1731		-13.149	4.403	1.00 52.20
MOTA	2401	SD	MET	1731		-14.840	3.994	1.00 64.38
MOTA	2402	CE	MET	1731	32.926	-14.502	2.606	1.00 63.03
MOTA	2403	C	MET	1731	29.992	-10.869	5.695	1.00 34.53
MOTA	2404	0	MET	1731		-10.268	4.619	1.00 35.08
MOTA	2405	N	MET	1732	28.971	-11.153	6.501	1.00 33.32

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MOTA 2407 CA MET 1732 27.594 -10.770 6.194 1.00 31.78 MOTA 2408 CB MET 1732 26.634 -11.346 7.236 1.00 30.42 MOTA 2409 CG MET 1732 25.172 -11.071 6.938 1.00 30.28 MOTA 2410 SD MET 1732 24.071 -11.709 8.183 1.00 27.41 **ATOM** 2411 CE MET 1732 23.738 -13.369 7.471 1.00 22.35 **ATOM** 2412 C MET 1732 27.484 -9.243 6.158 1.00 31.10 **ATOM** 2413 0 MET 1732 26.794 -8.680 5.303 1.00 31.08 ATOM 2414 N MET 1733 28.139 -8.586 7.114 1.00 31.22 **ATOM** 2416 CA MET 1733 28.161 -7.128 7.189 1.00 30.93 ATOM 2417 CB MET 1733 29.001 -6.665 8.376 1.00 31.91 ATOM 2418 CG MET 1733 28.368 -6.906 9.710 1.00 33.63 **ATOM** 2419 SD MET 1733 29.375 -6.210 11.021 1.00 34.53 ATOM 2420 CE MET 1733 29.106 -7.395 12.280 1.00 34.12 **ATOM** 2421 C 28.830 -6.623 MET 1733 5.921 1.00 32.49 MOTA 2422 O MET 1733 28.357 -5.682 5.281 1.00 33.61 MOTA 2423 N ARG 1734 29.932 -7.269 5.551 1.00 32.11 MOTA 2425 CA ARG 1734 30.673 -6.889 4.355 1.00 31.13 **ATOM** 2426 CB ARG 1734 32.012 -7.623 4.308 1.00 28.68 ATOM 2427 CG ARG 1734 32.953 -7.267 5.451 1.00 27.19 **ATOM** 2428 CD ARG 1734 33.159 -5.766 5.558 1.00 26.80 MOTA ARG 2429 NE 1734 4.393 1.00 35.67 33.864 -5.243 MOTA 2431 CZ ARG 4.223 1.00 38.03 1734 35.187 -5.305 MOTA 2432 NH1 ARG 1734 35.967 -5.861 5.148 1 00 38.07 ATOM 2435 NH2 ARG 1734 35.729 -4.850 3.094 1.00 38.87 MOTA 2438 C ARG 1734 29.873 3.065 1.00 29.53 -7.098 **ATOM** 2439 O ARG 1734 30.029 -6.334 2.121 1.00 29.11 ATOM 2440 N ASP 1735 29.036 -8.137 3.025 1.00 29.48 ATOM 2442 CA ASP 1735 28.193 -8.412 1.859 1.00 26.82 ATOM 2443 CB ASP 1735 27.591 -9.811 1.933 1.00 30.25 ATOM 2444 CG ASP 1735 28.632 -10.895 1.773 1.00 35.13 MOTA 2445 OD1 ASP 1735 29.626 -10.645 1.052 1.00 35.19 MOTA 2446 OD2 ASP 1735 28.458 -11.990 2.366 1.00 39.35 MOTA 2447 C ASP 1.735 27.082 -7.375 1.760 1.00 23.88 MOTA 2448 O ASP 1735 26.692 --6.992 0.656 1.00 24.83 A'TOM 2449 N CYS 1736 26.574 -6.929 2.913 1.00 22.13 **ATOM** 2451 CA CYS 1736 25.538 -5.887 2.965 1.00 21.74 ATOM 1736 2452 CB CYS 25.005 -5.692 4.401 1.00 20.46 MOTA 2453 SG CYS 1736 23.978 -7.013 5.053 1.00 19.59 ATOM 2454 C CYS 1736 26.104 -4.542 2.456 1.00 20.51 **ATOM** 2455 0 CYS 1736 25.377 -3.732 1.887 1.00 16.07 **ATOM** 2456 N TRP 1737 27.401 -4.325 2.670 1.00 21.58 MOTA 2458 CA TRP 1737 28.080 -3.113 2.248 1.00 20.57 MOTA 2459 CB TRP 1737 29.107 -2.682 3.291 1.00 17.02 MOTA 2460 CG TRP 1737 28.558 -2.415 4.654 1.00 20.35 MOTA 2461 CD2 TRP 1737 29.254 -2.564 5.897 1.00 20.42 MOTA 2462 CE2 TRP 1737 28.387 -2.122 6.923 1.00 21.18 MOTA 2463 CE3 TRP 1737 30.538 -3.027 6.243 1.00 21.60 MOTA 2464 CD1 TRP 1737 27.317 -1.914 4.970 1.00 19.86 MOTA 2465 NE1 TRP 1737 27.210 -1.732 6.328 1.00 21.03 MOTA 2467 CZ2 TRP 1737 28.760 -2.125 8.276 1.00 21.70 MOTA 2468 CZ3 TRP -3.031 1737 30.910 7.594 1.00 21.73 ATOM 2469 CH2 TRP 1737 30.025 -2.584 8.588 1.00 23.06

MOTA	2470	С	TRP	1737	28.770	-3.281	0.899	1.00 24.98
ATOM	2471	0	TRP	1737	29.758	-2.607	0.610	1.00 25.84
ATOM	2472	N	HIS	1738	28.269	-4.185	0.063	1.00 27.61
MOTA	2474	CA	HIS	1738	28.885	-4.352	-1.243	1.00 25.81
ATOM	2475	CB	HIS	1738	28.263	-5.522	-2.013	1.00 24.74
ATOM	2476	CG	HIS	1738	29.105	-6.005	-3.162	1.00 26.07
ATOM	2477	CD2	HIS	1738	29.599	-5.353	-4.246	1.00 25.45
MOTA	2478	ND1	HIS	1738	29.571	-7.299	-3.252	1.00 24.60
ATOM	2480	CEl	HIS	1738	30.320	-7.422	-4.333	1.00 24.62
ATOM	2481	NE2	HIS	1738	30.352	-6.253	-4.954	1.00 23.97
MOTA	2483	С	HIS	1738	28.734	-3.034	-2.017	1.00 26.41
ATOM	2484	0	HIS	1738	27.705	-2.350	-1.931	1.00 25.20
MOTA	2485	N	ALA	1739	29.792	-2.658	-2 727	1.00 26.45
MOTA	2487	CA	ALA	1739	. 29.829	-1.437	-3.517	1.00 25.61
MOTA	2488	CB	ALA	1739	31.193	-1.285	-4.117	1.00 25.87
MOTA	2489	С	ALA	1739	28.765	-1.418	-4.617	1.00 26.67
ATOM	2490	0	ALA	1739	28.207	-0.367	-4.930	1.00 28.28
ATOM	2491	N	VAL	1740	28.529	-2.573	-5.235	1.00 25.10
ATOM	2493	CA	VAL	1740	27.526	-2.706	6.292	1.00 24.14
MOTA	2494	CB	VAL	1740	27.969	-3.737	-7.378	1.00 24.27
ATOM	2495	CG1	VAL	1740	26.979	-3.792	-8.503	1.00 20.03
ATOM	2496	CG2	VAL	1740	29.331	-3.375	-7.926	1.00 26.74
ATOM	2497	C	VAL	1740	26.234	-3.196	-5.639	1.00 23.91
ATOM	2498	0	VAL	1740	26:173	-4.349	-5.175	1.00 26.37
ATOM	2499	N	PRO	1741	25.173	-2.357	-5.653	1.00 24.55
ATOM	2500	CD	PRO	1741	25.096	-1.065	-6.369	1.00 17.73
ATOM	2501	CA	PRO	1741	23.868	-2.686	-5.058	1.00 22.27
MOTA	2502	CB	PRO	1741	22.979	-1.536	-5.545	1.00 17.82
MOTA	2503	CG	PRO	1741	23.925	-0.410	-5.710	1.00 13.27
ATOM	2504	C	PRO	1741	23.275	-4.057	-5.418	1.00 24.04
ATOM	2505	0	PRO	1741	22.735	-4.748	-4.548	1.00 25.86
ATOM	2506	N	SER	1742	23.431	-4.471	-6.674	1.00 24.30
MOTA	2508	CA	SER	1742	22.888	-5.745	-7.167	1.00 24.42
ATOM	2509	CB	SER	1742	22.986	-5.819	-3.696	1.00 23.95
ATOM	2510	OG	SER	1742	24.334	-5.784	-9.131	1.00 22.98
ATOM	2512	С	SER	1742	23.553	-6.978	-6.589	1.00 25.20
ATOM	2513	0	SER	1742	22.994	-8.085	-6.677	1.00 23.68
ATOM	2514	N	GLN	1743	24.753	-6.793	-6.037	1.00 25.46
ATOM	2516	CA	GLN	1743	25.504	-7.910	-5.485	1.00 25.64
ATOM	2517	CB	GLN	1743	26.993	-7.773	-5.807	1.00 24.02
ATOM	2518	CG	GLN	1743	27.263	-7.768	-7.295	1.00 22.75
ATOM	2519	CD	GLN	1743	26.585	-8.938	-8.014	1.00 26.21
ATOM	2520	OE1		1743	26.999	-10.087	-7.864	1.00 28.67
ATOM	2521	NE2	GLN	1743	25.535	-8.649	-8.787	1.00 21.57
ATOM	2524	С	GLN	1743	25.270	-8.148	-4.007	1.00 24.86
ATOM	2525	0	GLN	1743	25.685	-9.173	-3.456	1.00 25.24
ATOM	2526	N	ARG	1744	24.525	-7.244	-3.389	1.00 23.38
ATOM	2528	CA	ARG	1744	24.230	-7.376	-1.976	1.00 22.41
ATOM	2529	CB	ARG	1744	23.727	-6.055	-1.415	1.00 22.24
ATOM	2530	CG	ARG	1744	24.718	-4.909	-1.523	1.00 22.53
MOTA	2531	CD	ARG	1744	24.084	-3.577	-1.134	1.00 19.82
ATOM	2532	NE	ARG	1744	24.963	-2.475	-1.517	1.00 22.51

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ATOM 2534 CZARG 1744 -1.201 -1.663 24.592 1.00 22.92 **ATOM** 2535 NH1 ARG 1744 23.332 -0.814 -1.458 1.00 18.28 MOTA 2538 NH2 ARG 1744 25.491 -0.310 -2.060 1.00 22.15 **ATOM** 2541 C ARG 1744 23.163 -8.458 -1.833 1.00 24.61 MOTA 2542 0 ARG 1744 22.428 -8.755 -2.786 1.00 26.94 **ATOM** 2543 N PRO 1745 23.143 -9.155 -0.688 1.00 23.21 MOTA CD PRO 2544 1745 24.052 -9.107 0.470 1.00 22.38 MOTA 2545 CA PRO 1745 22.129 -10.190 -0.522 1.00 22.24 MOTA 2546 CB PRO 1745 22.623 -10.942 0.711 1.00 21.13 MOTA 2547 CG PRO 1745 23.286 -9.864 1.504 1.00 20.24 2548 ATOM C 1745 PRO 20.800 -9.506 -0.256 1.00 23.11 . MOTA 2549 0 PRO 1745 20.743 -8.300 0.020 1.00 25.93 **ATOM** 2550 N THR 1746 19.724 -10.256 -0.373 1.00 20.82 **ATOM** 2552 CA THR 1746 18.420 -9.697 -0.112 1.00 20.47 MOTA 2553 CB THR 1746 17..386 -10.342 -1.041 1.00 18.61 MOTA 2554 OG1 THR 1746 17.382 -11.755 -0.822 1.00 21.86 MOTA 2556 CG2 THR 1746 17.746 -10.078 -2.487 1.00 21.13 **ATOM** 2557 C THR 1746 18.060 -9.970 1.344 1.00 20.84 MOTA 2558 0 THR 1746 18.787 -10.674 2.055 1.00 22.08 MOTA 2559 N PHE 1747 16.953 -9.406 1.810 1.00 21.58 **ATOM** 2561 CA PHE 1747 16.536 -9.675 3.178 1.00 21.15 **ATOM** 2562 ĊВ PHE 1747 15.442 -8.710 3.613 1.00 20 34 2563 **ATOM** CG PHE 1747 15.961 -7.350 3.982 1.00 23.18 ATOM 2564 CD1 PHE 1747 -7 170 16.729 5.130 1.00 22.26 MOTA 2565 CD2 PHE -6.240 1747 15.668 3.196 1.00 23.41 MOTA 2566 PHE CE1 .1747 17.186 -5.909 5.484 1.00 17.31 **ATOM** 2567 CE2 PHE 1747 -4.967 16.124 3.548 1.00 17.93 ATOM 2568 CZ PHE 1747 16.883 -4.809 4.696 1.00 19.06 MOTA 2569 С PHE 1747 Lo.062 -11.124 3.217 1.00 21.51 MOTA 2570 O PHE 1747 16.248 -11.823 4.212 1.00 22.19 ATOM 2571 N LYS 1748 15.490 -11.588 2.111 1.00 22.00 MOTA 2573 CA LYS 1748 15.048 -12.973 2.009 1.00 24.34 MOTA 2574 CB LYS 1748 14.471 -13.227 0.621 1.00 23.61 **ATOM** 2575 CG LYS 1748 14.050 -14.663 0.416 1.00 27.45 MOTA. 2576 CD LYS 1748 13.633 -14.932 -0.998 1.00 28.97 MOTA 2577 CE LYS 174B 13.244 -16.394 -1.163 1.00 35.95 MOTA 2578 NZ LYS 1748 12.213 -16.795 -0.153 1.00 41.69 MOTA 2582 C LYS 174B 16.257 -13.907 2.264 1.00 27.58 MOTA 2583 0 LYS 1748 16.161 -14.863 3.034 1.00 29.73 MOTA 2584 GLN 1749 N 17.397 -13.604 1.640 1.00 25.88 **ATOM** 2586 CA GLN 1749 18.617 -14.394 1.804 1.00 23.72 ATOM 2587 CB GLN 1749 19.692 -13.925 0.837 1.00 27.00 **ATOM** 2588 CG GLN 1749 19.338 -13.954 -0.628 1.00 32.28 **ATOM** 2589 CD GLN 1749 20.442 -13.331 -1.477 1.00 36.35 MOTA 2590 OE1 GLN 1749 20.175 -12.528 -2.368 1.00 37.63 ATOM 2591 NE2 GLN 1749 21.699 -13.702 -1.194 1.00 38.60 **ATOM** 2594 GLN C 1749 19.177 -14.266 3.212 1.00 23.44 **ATOM** 2595 0 GLN 1749 19.586 -15.260 3.826 1.00 23.52 **ATOM** 2596 LEU N 1750 19.267 -13.035 3.703 1.00 21.73 ATOM 2598 CA LEU 1750 19.787 -12.796 5.054 1.00 20.90 ATOM 2599 CB LEU 1750 19.752 -11.308 5.359 1.00 18.60 **ATOM** 2600 CG LEU 1750 20.654 -10.439 4.485 1.00 16.53

ATOM	2601	CD1	LEU	1750	20.190	-8.979	4.579	1.00 13.28
ATOM	2602		LEU	1750	22.100	-10.612	4.939	1.00 14.74
ATOM	2603	С	LEU	1750	18.982	-13.548	6.108	1.00 21.25
MOTA	2604	0	LEU	1750	19.534	-14.056	7.084	1.00 21.26
ATOM	2605	N	VAL	1751	17.671	-13.607	5.917	1.00 21.64
ATOM	2607	CA	VAL	1751	16.793	-14.289	6.845	1.00 21.21
MOTA	2608	CB	VAL	1751	15.353	-14.072	6.432	1.00 19.03
MOTA	2609	CG1	VAL	1751	14.453	-14.970	7.220	1.00 23.34
ATOM	2610	CG2	VAL	1751	14.978	-12.648	6.684	1.00 22.78
MOTA	2611	С	VAL	1751	17.127	-15.774	6.925	1.00 25.56
MOTA	2612	0	VAL	1751	17.111	-16.369	8.007	1.00 25.61
ATOM	2613	N	GLU	1752	17.418	-16.381	5.778	1.00 28.61
ATOM	2615	CA	GLU	1752	17.773	-17.789	5.755	1.00 32.38.
MOTA	2616	CB	GLU	1752	17.765	-18.317	4.321	1.00 37.26
ATOM	2617	CG	GLU	1752	16.399	-18.218	3.651	1.00 44.76
ATOM	2618	CD	GLU	1752	16.394	-18.742	2.219	1.00 50.37
ATOM	2619	OE1	GLU	1752	15.397	-18.495	1.497	1.00 52.52
ATOM	2620	OE2	GLU	1752	17.377	-19.410	1.822	1.00 51.96
MOTA	2621	C	GLU	1752	19.140	-17.984	6.405	1 00 32.27
ATOM	2622	0	GLU	1752	19.330	-18.878	7.237	1.00 31.18
ATOM	2623	N	ASP	1753	20.069	-17.096	6.083	1.90 33.20
ATOM	2625	CA	ASP	1753	21.411	-17.174	6.547	1.00 35.13
ATOM	2626	СВ	ASP	1753	22.341	-16.144	5.998	1.00 37 80
ATOM	2627	CG	ASP	1753	22.498	-16.358	4.502	1.00 41.13
MOTA	2628	OD1		1753	22.222	-17.470	4.007	1.00 43.01
MOTA	2629	OD2	ASP	1753	22.908	-15.401	3.811	1.00 44.26
ATOM	2630	C	ASP	1753	21.379	-16.986	8.153	1.00 33.84
MOTA	2631	0	ASP	1753	21.971	-17.773	8.901	1.00 36.22
ATOM	2632	N	LEU	1754	20.652	-15.978	8.633	1.00 30.73
ATOM	2634	CA	LEU	1754	20.568	-15.730	10.070	1.00 28.51
ATOM	2635	CB	LEU	1754	19.881	-14.394	10.355	1.00 25.20
ATOM	2636	CG	LEU	1754	20.810	-13.225	10.016	1.00 26.72
ATOM	2637	CD1		1754		-11.903	9.905	1.00 24.18
MOTA	2638	CD2		1754		-13.168	11.063	1.30 25.€9
MOTA	2639	С	LEU	1754		-16.870	10.763	1.00 28.74
ATOM	2640	0	LEU	1754		-17.290	11.832	1.00 29.08
ATOM	2641	N	ASP	1755		-17.419	10.130	1.00 29.97
ATOM	2643	CA	ASP	1755		-18.519	10.732	1.00 31.58
MOTA	2644	CB	ASP	1755		-18.930	9.843	1.00 36.47
MOTA	2645	CG	ASP	1755		-20.005	10.467	1.00 39.40
ATOM	2646	OD1		1755		-19.869	11.651	1.00 45.91
ATOM	2647	OD2		1755		-20.995	9.774	1.00 45.68
ATOM	2648	C	ASP	1755		-19.703	10.952	1.00 32.29
ATOM	2649			1755		-20.380	11.979	1.00 31.66
ATOM	2650		ARG	1756		-19.923	9.989	1.00 32.32
ATOM	2652		ARG	1756		-21.015	10.059	1.00 32.73
ATOM	2653	CB	ARG	1756		-21.145	8.704	1.00 34.47
ATOM	2654	CG	ARG	1756		-22.157	8.645	1.00 37.78
ATOM	2655	CD	ARG	1756		-22.274	7.237	1.00 43.87
ATOM	2656	NE	ARG	1756		-20.999	6.702	1.00 48.78
ATOM	2658	CZ	ARG	1756		-20.380	7.122	1.00 52.92
ATOM	2659	NH1	AKG	1756	25.630	-20.914	8.091	1.00 55.88

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MOTA 2662 NH2 ARG 1756 6.593 1.00 52.53 25.237 -19.214 MOTA ARG 2665 C 1756 21.889 -20.761 11.186 1.00 33.76 MOTA 2666 0 ARG 1756 22.131 -21.619 12.049 1.00 34.53 ATOM 2667 N ILE 1757 22.432 -19.553 11.204 1.00 33.49 **ATOM** 2669 CA ILE 1757 23.405 -19.176 12.205 1.00 32.71 **ATOM** 2670 CB ILE 1757 23.980 -17.764 11.919 1.00 31.86 **ATOM** 2671 CG2 ILE 1757 25.111 -17.454 12.869 1.00 31.71 **ATOM** 2672 CG1 ILE 1757 24.520 -17.704 10.488 1.00 31.41 **ATOM** 2673 CD1 ILE 1757 25.075 -16.366 10.096 1.00 27.68 ΜΟΤΛ 2674 C ILE 1757 22.807 -19.236 13.604 1.00 34.20 MOTA 2675 O ILE 23.399 -19.833 1757 14.495 1.00 35.83 **ATOM** 2676 N VAL 1758 1 21.620 -18.667 13.792 1.00 35.40 VAL ATOM 2678 CA 1758 20.981 -18.653 15.108 1.00 37.49 **ATOM** 2679 CB VAL 1758 19.501 -18.160 15.061 1.00 34.42 **ATOM** 2680 CG1 VAL 175B 18.899 -18.199 16.456 1.00 37.37 ATOM 2681 CG2 VAL 1758 19.403 -16.742 14.519 1.00 30.02 MOTA 2682 С VAL 1758 21.010 -20.050 15.715 1.00 41.64 MOTA 2683 VAL 1758 0 21.533 -20.246 16.817 1.00 43.69 **ATOM** 2684 ALA 1759 N 20.492 -21.015 14 961 1.00 44.52 MOTA 2686 CA ALA 1759 20.434 -22.415 15.387 1.00 45.20 MOTA 2687 CB ALA 1759 19.833 -23.268 14.277 1.00 43.44 **ATOM** 2688 C ALA 1759 21.791 -22.968 15.795 1.00 45.91 **ATOM** 2689 0 ALA 1759 21.890 -23.780 16.710 1.00 47.41 ATOM 2690 N LEU 1760 22.833 -22.511 15.120 1.00 47.70 **ATOM** 2692 CA LEU 1760 24.190 -22.960 15.399 1.00 50.91 **ATOM** 2693 LEU CB 1760 25.015 -22.912 14.109 1.00 52.93 ATOM 2694 LEU CG 1760 24.448 -23.723 12.947 1.00 57.55 MOTA 2695 CD1 LEU 1760 25.189 -23.390 11,660 1.00 60.76 MOTA 2696 CD2 LEU 1760 24.539 -25.208 13.273 1.00 58.66 **ATOM** 2697 C LEU 1760 24.882 -22.111 16.472 1.00 52.07 **ATOM** 2698 O LEU 1760 25.967 -22.459 16.953 1.00 51.95 24.267 -21.000 ATOM 2699 N THR 1761 16.850 1.00 52.05 **ATOM** 2701 CA THR 1761 24.868 -20.131 17.836 1.00 53.28 ATOM 2702 CB THR 1761 24.362 -18.693 17.673 1.00 54.58 **ATOM** 2703 OG1 THR 1761 24.633 -18.259 16.339 1.00 53.68 **ATOM** 2705 CG2 THR 1761 25.090 -17.762 18.621 1.00 55.45 24.715 -20.619 MOTA 2706 C THR 1761 19.272 1.00 53.31 **ATOM** 2707 O THR 1761 23.629 -20.986 19.713 1.00 53.89 ATOM 2708 N SER 1762 25.832 -20.617 19.993 1.00 53.51 MOTA 2710 CA SER 1762 25.876 -21.045 21.383 1.00 53.15 MOTA SER 2711 CB 1762 27.340 -21.131 21.830 1.00 57.27 MOTA OG SER 2712 1762 27.492 -21.872 23.028 1.00 61.22 ATOM С SER 2714 1762 25.110 -20.048 22.257 1.00 49.15 MOTA 2715 0 SER 1762 25.229 -18.831 22.071 1.00 46.61 MOTA 3466 N ALA 461 79.636 26.047 14.493 1.00 61.05 **ATOM** 3468 CA ALA 79.609 24.852 461 13.654 1.00 58.10 **ATOM** 3469 CB ALA 461 78.335 24.024 13.935 1.00 60.39 **ATOM** 3470 С ALA 461 79.694 25.239 12.179 1.00 54.65 **ATOM** 3471 0 ALA 461 79.653 24.382 11.297 1.00 54.05 **ATOM** 3472 N ALA 462 79.867 26.537 11.935 1.00 51.68 MOTA 3474 CA ALA 462 79.972 27.085 10.584 1.00 48.47 MOTA 3475 CB ALA 462 80.099 28.619 10.633 1.00 46.99

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MOTA	3476	С	ALA	462	81.123	26.489	9.766	1.00 44.86
ATOM	3477	0	ALA	462	80.918	26.097	8.625	1.00 43.40
MOTA	3478	N	TYR	463	82.329	26.447	10.335	1.00 42.23
ATOM	3480	CA	TYR	463	83.493	25.913	9.629	1.00 39.04
ATOM	3481	CB	TYR	463	84.642	26. 9 21	9.620	1.00 39.01
ATOM	3482	CG	TYR	463	84.354	28.126	8.743	1.00 41.95
ATOM	3483	CD1	TYR	463	84.073	29.373	9.308	1.00 42.40
MOTA	3484	CE1	TYR	463	83.754	30.466	8.512	1.00 42.02
MOTA	3485	CD2	TYR	463	84.311	28.009	7.345	1.00 40.70
MOTA	3486	CE2	TYR	463	83.992	29.099	6.542	1.00 37.09
ATOM	3487	CZ	TYR	463	83.716	30.320	7.134	1.00 39.19
ATOM	3488	ОН	TYR	463	83.401	31.406	6.360	1.00 40.66
ATOM.	3490	C	TYR	463	84.011	24.554	10.050	1.00 37:78
ATOM	3491	0	TYR	463	84.627	23.863	9.237	1.00 38.35
ATOM	3492	N	GLU	464	83.746	24.143	11.285	1.00 37.67
ATOM	3494	CA	GLU	464	84.212	22.841	11.747	1.00 38.57
ATOM	3495	CB	GLU	464	85.707	22.890	12.024	1.00 41.44
ATOM	3496	CG	GLU	464	86.093	23.870	13.108	1.00 47.87
MOTA	3497	CD	GLU	464	87.583	24.135	13.169	1.00 53.44
MOTA	3498		GLU	464	87.998	24.983	13.990	1.00 56.72
ATOM	3499	OE2	GLU	464 .	88.344	23.513	12.397	1.00 54.85
ATOM	3500	C	GLU	464	83.504	22.393	13.001	1.00 38.15
ATOM	3501	0	GLU	464	83.291	23.187	13.905	1.00 39.59
ATOM	3502	N	LEU	465	83.121	21.124	13.051	1.00 37.13
ATOM	3504	CA	LEU	465	82.457	20.608	14.236	1 00 37.93
ATOM	3505	CB	LEU	465	81.502	19.456	13.894	1.00 33.43
ATOM	3506	CG	LEU	465	80.455	19.609	12.787	1.00 31.12
MOTA	3507	CD1		465	79.415	18.500	12.944	1.00 24.85
ATOM	3508	CD2		465	79.797	20.980	12.855	1.00 29.05
MOTA	3509	C	LEU	465	83.540	20.090	15.166	1.00 41.02
ATOM	3510	0	LEU	465	84.703	19.93€	14.763	1.00 40.24
ATOM	3511	N	PRO	466	83.198	19.884	16.441	1.00 43.58
ATOM	3512	CD	PRO	466	81.974	20.359	17.115	1.00 45.33
ATOM	3513	CA	PRO	466	84.170	19.374	17.415	1.00 44.72
ATOM	3514	CB	PRO	466	83.433	19.505	18.743	1.00 46.18
ATOM ATOM	3515	CG	PRO	466	82.486	20.679	18.496	1.00 48.84
ATOM	3516	C	PRO	466	84.447	17.909	17.101	1.00 44.52
ATOM	3517	0	PRO	466	83.616	17.228	16.509	1.00 43.38
ATOM	3518	N	GLU	467	85.610	17.421	17.492	1.00 47.75
	3520	CA	GLU	467	85.932	16.035	17.218	1.00 51.03
ATOM ATOM	3521 3522	CB CG	GLU	467	87.354	15.913	16.659	1.00 56.11
ATOM	3523		GLU	467	87.615	14.557	16.000	1.00 62.27
ATOM			GLU	467	88.927	14.489	15.242	1.00 66.39
ATOM		OE1 OE2		467	89.688	15.490	15.243	1.00 69.85
ATOM			GLU	467	89.182	13.418	14.643	1.00 66.09
ATOM	3526 3527		GLU	467	85.749	15.136	18.435	1.00 49.62
ATOM ATOM			GLU	467 468	85.767	15.601	19.578	1.00 49.62
ATOM			ASP		85.516	13.856	18.166	1.00 48.07
ATOM			ASP	468	85.352	12.843	19.198	1.00 46.32
			ASP	468	83.880	12.679	19.587	1.00 45.15
			ASP	468	83.678	11.740	20.779	1.00 44.19
ATOM	3533	OD1	ASP	468	82.544	11.709	21.309	1.00 42.04

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MOTA	3534	OD2	ASP	468	84.629	11.033	21.188	1.00 38.14
ATOM	3535	C	ASP	468	85.877	11.556	18.580	1.00 45.54
MOTA	3536	0	ASP	468	85.141	10.815	17.928	1.00 45.94
ATOM	3537	N	PRO	469	87.181	11.308	18.732	1.00 45.89
ATOM	3538	CD	PRO	469	88.111	12.189	19.464	1.00 45.11
ATOM	3539	CA	PRO	469	87.885	10.130	18.215	1.00 45.91
MOTA	3540	CB	PRO	469	89.208	10.187	18.968	1.00 45.90
ATOM	3541	CG	PRO	469	89.456	11.662	19.042	1.00 45.73
ATOM	3542	С	PRO	469	87.170	8.806	18.473	1.00 45.48
ATOM	3543	0	PRO	469	87.188	7.905	17.629	1.00 46.83
ATOM	3544	N	ARG	470	86.495	8.717	19.613	1.00 42.12
ATOM	3546	CA	ARG	470	85.786	7.506	19.999	1.00 41.21
ATOM	35 <u>4</u> 7	CB	ARG	470	85.083	7.704	21.331	1.00 43.14
MOTA	3548	CG	ARG	470	85.885	8.424	22.375	1.00 45.68
ATOM	3549	CD	ARG	470	85.014	8.705	23.564	1.00 45.98
ATOM	3550	NE	ARG	470	83.802	9.417	23.184	1.00 47.28
ATOM	3552	CZ	ARG	470	82.921	9.877	24.057	1.00 50.54
ATOM	3553	NHl	ARG	470	83.127	9.687	25.354	1.00 47.56
ATOM	3556	NH2	ARG	470	81.843	10.527	23 637	1.00 54.59
ATOM	3559	C	ARG	470	84.736	7.058	19.004	1.00 40.57
ATOM	3560	0	ARG	470	84.411	5.877	18.941	1.00 43.13
ATOM	3561	N	TRP	471	84.182	8.014	18.268	1.00 38.07
ATOM	3563	CA	TRP	471	83.124	7.736	17.314	1.00 35.09
MOTA	3564	CB	TRP	471	81.890	8.515	17.739	1.00 33.42
ATOM	3565	CG	TRP	471	81.259	7.958	18.952	1.00 31.71
MOTA	3566	CD2	TRP	471	80.512	6.740	19.026	1.00 34.81
MOTA	3567	CE2	TRP	471	80.061	6.610	20.355	1.00 33.17
MOTA	3568		TRP	471	80.174	5.744	18.092	1.00 37.60
MOTA	3569		TRP	471	81.246	8.503	20.199	1.00 25.70
ATOM	3570	NEl		471	80.525	7.697	21.051	1.00 28.79
MOTA	3572	CZ2	TRP	471	79.289	5.522	20.776	1.00 35.80
ATOM	3573	CZ3	TRP	471	79.409	4.660	18.509	1.00 35.52
MOTA	3574	CH2	TRP	471	78.973	4.560	19.839	1.00 34.51
ATOM	3575	С	TRP	471	83.432	8.065	15.872	1.00 35.77
ATOM	3576	0	TRP	471	82.690	7.670	14.968	1.00 37.45
ATOM	3577	N	GLU	472	84.533	8.770	15.651	1.00 34.76
MOTA	3579	CA	GLU	472	84.895	9.184	14.308	1.00 34.51
MOTA	3580	СВ	GLU	472	86.065	10.174	14.365	1.00 32.30
MOTA	3581	CG	GLU	472	86.221	11.038	13.103	1.00 36.57
ATOM	3582	CD	GLU	472	85.082	12.035	12.872	1.00 36.34
ATOM ATOM	3583	OE1		472	84.515	12.558	13.857	1.00 36.01
	3584	OE2		472	84.777	12.318	11.694	1.00 31.95
MOTA	3585	С	GLU	472	85.219	8.034	13.364	1.00 33.90
ATOM	3586	0	GLU	472	85.896	7.082	13.745	1.00 33.77
ATOM	3587	N	LEU	473	84.667	8.094	12.158	1.00 33.58
ATOM	3589	CA	LEU	473	84.944	7.095	11.146	1.00 34.82
MOTA	3590	CB	LEU	473	83.714	6.234	10.847	1.00 32.59
MOTA	3591	CG	LEU	473	84.020	5.091	9.867	1.00 33.78
MOTA	3592	CD1		473	84.786	4.000	10.578	1.00 32.94
MOTA	3593	CD2		473	82.759	4.518	9.273	1.00 35.34
ATOM	3594		LEU	473	85.380	7.828	9.883	1.00 37.95
ATOM	3595	0	LEU	473	84.720	8.781	9.457	1.00 39.55

ATOM	3596	N	PRO	474	86.522	7.423	9.299	1.00 38.99
ATOM	3597	CD	PRO	474	87.455	6.453	9.899	1.00 38.76
ATOM	3598	CA	PRO	474	87.094	8.004	8.080	1.00 39.37
MOTA	3599	CB	PRO	474	88.382	7.201	7.906	1.00 40.18
MOTA	3600	CG	PRO	474	88.767	6.883	9.310	1.00 37.76
ATOM	3601	С	PRO	474	86.165	7.794	6.890	1.00 40.94
ATOM	3602	0	PRO	474	85.865	6.653	6.532	1.00 43.98
ATOM	3603	N	ARG	475	85.762	8.886	6.245	1.00 40.66
MOTA	3605	CA	ARG	475	84.850	8.840	5.101	1.00 40.66
MOTA	3606	CB	ARG	475	84.776	10.216	4.448	1.00 37.94
ATOM	3607	CG	ARG	475	84.354	11.300	5.415	1.00 36.12
MOTA	3608	CD	ARG	475	84.340	12.697	4.800	1.00 35.92
MOTA	3609	NE	ARG	475	83.932	13.677	5.801	1.00 30.14
ATOM	3611	CZ	ARG	475	82.671	13.878	6.170	1.00 28.45
MOTA	3612	NH1	ARG	475	81.689	13.197	5.599	1.00 28.41
MOTA	3615	NH2	ARG	475	82.410	14.666	7.197	1.00 27.85
MOTA	3618	С	ARG	475	85.141	7.766	4.046	1.00 41.44
MOTA	3619	0	ARG	475	84.223	7.189	3.470	1.00 41.40
MOTA	3620	N	ASP	476	86.419	7.475	3.830	1.00 44.99
MOTA	3622	CA	ASP	476	86.836	6.477	2.849	1.00 50.62
ATOM	3623	CB	ASP	476	88.344	6.540	2.644	1.00 54.47
MOTA	3624	CG	ASP	476	89.105	5.969	3.819	1.00 60.03
MOTA	3625	OD1	ASP ·	476	. 89.569	4.810	3.722	1.00 65.09
ATOM	3626	OD2	ASP	476	89.216	6.669	4.846	1.00 62.62
ATOM	3627	С	ASP	476	86.436	5.054	3.263	1.00 51.16
MOTA	3628	0	ASP	476	86.678	4.091	2.530	1.00 53.06
MOTA	3629	N	ARG	477	85.900	4.916	4.471	1.00 49.58
ATOM	3631	CA	ARG	47?	85.443	3.623	4.968	1.00 47.34
ATOM	3632	CB	ARG	477 .	86.040	3.359	6.341	1.00 48.85
ATOM	3633	CG	ARG	477	87.481	2.924	6.265	1.00 52.11
MOTA	3634	CD	ARG	477	88.169	3.079	7.591	1.00 53.63
MOTA	3635	NE	ARG	477	87.515	2.345	8.665	1.00 54.86
ATOM	3637	CZ	ARG	477	87.932	2.363	9.927	1.00 57.15
MOTA	3638		ARG	477	89.000	3.076	10.264	1.00 55.98
MOTA	3641		ARG	477	87.269	1.691	10.855	1.00 58.31
MOTA	3644	С	ARG	47 7	83.915	3.563	5.020	1.00 44.70
MOTA	3645	0	ARG	477	83.339	2.780	5.770	1.00 44.63
MOTA	3646	N	LEU	478	83.274	4.366	4.179	1.00 41.95
MOTA	3648	CA	LEU	478	81.832	4.440	4.118	1.00 38.58
MOTA	3649	CB	LEU	478	81.374	5.609	4.980	1.00 33.17
ATOM	3650	CG	LEU	478	79.872	5.731	5.183	1.00 29.07
ATOM	3651		LEU	478	79.393	4.592	6.052	1.00 28.25
ATOM	3652		LEU	478	79.590	7.059	5.836	1.00 30.79
ATOM	3653	С	LEU	478	81.432	4.710	2.674	1.00 38.93
ATOM	3654	0	LEU	478	81.938	5.647	2.071	1.00 41.75
ATOM	3655	N	VAL	479	80.562	3.880	2.107	1.00 37.96
MOTA	3657	CA	VAL	479	80.113	4.086	0.730	1.00 37.87
ATOM	3658	CB	VAL	479	80.468	2.882	-0.192	1.00 36.47
ATOM	3659		VAL	479	80.001	3.145	-1.612	1.00 34.43
ATOM	3660		VAL	479	81.972	2.651	-0.187	1.00 34.33
MOTA	3661	С	VAL	479	78.609	4.299	0.775	1.00 38.10
MOTA	3662	0	VAL	479	77.846	3.366	1.019	1.00 40.13

ATOM	3663	N	LEU	480	78.184	5.537	0.552	1.00 38.05
ATOM	3665	CA	LEU	480	76.766	5.879	0.606	1.00 35.90
MOTA	3666	CB	LEU	480	76.568	7.393	0.475	1.00 33.98
ATOM	3667	CG	LEU	480	77.276	8.257	1.536	1.00 32.84
ATOM	3668	CD1	LEU	480	77.003	9.749	1.273	1.00 29.68
ATOM	3669	CD2	LEU	480	76.828	7.861	2.943	1.00 26.03
MOTA	3670	С	LEU	480	76.015	5.146	-0.476	1.00 34.99
MOTA	3671	0	LEU	480	76. 5 73	4.864	-1.526	1.00 36.12
ATOM	3672	N	GLY	481	74.753	4.836	-0.223	1.00 35.21
MOTA	3674	CA.	GLY	481	73.965	4.120	-1.204	1.00 34.79
ATOM	3675	C	GLY	481	72.544	4.608	-1.332	1.00 36.31
ATOM -	3676	0	GLY	481	72.237	5.775	-1.046	1.00 38.30
MOTA	3677	N	LYS	482	71.665	3.705	-1.761	1.00 35.59
MOTA	3679	CA	LYS	482	70.257	4.007	-1.959	1.00 35.24
ATOM	3680	CB	LYS	482	69.488	2.698	-2.207	1.00 35.69
ATOM	3681	С	LYS	182	69.585	4.763	-0.823	1.00 36.31
MOTA	3682	0	LYS	482	69.752	4.421	0.352	1.00 34.90
ATOM	3683	N	PRO	483	68.787	5.786	-1.157	1.00 38.08.
MOTA	3684	CD	PRO	483	68.432	6.320	-2.483	1.00 39.57
ATOM	3685	CA	PRO	483	68.097	6.566	-0.135	1.00 41.08
ATOM	3686	CB	PRO	483 .	67.300	7.560	-0.987	1.00 39.80
ATOM	3687	CG	PRO	483	68.268	7.819	-2.157	1.00 37.87
ATOM	3688	C	PRO	483	67.130	5.652	0.606	1.00 42.11
MOTA	3689	0	PRO	483	66.306	4.994	-0.025	1.00 43 01
A.TOM	3690	N	LEU	484	67.199	5.624	1.937	1.00 41.06
ATOM	3692	CA	LEU	484	66.293	4.823	2.751	1.00 38.47
ATOM	3693	CB	LEU	484	67.040	4.307	3.990	1.00 32.45
MOTA	3694	CG	LEU	484	67.968	3.098	3.809	1.00 27.68
ATOM	3695	CD1	LEU	484	68.569	2.710	5.147	1.00 20.29
ATOM	3696	CD2	LEU	484	67.181	1.964	3.225	1.00 23.20
MOTA	3697	С	LEU	484	65.084	5.637	3.180	1.00 42.18
MOTA	3698	O	LEU	484	65.227	6.699	3.814	1.00 44.50
MOTA	3699	Ŋ	GLY	485	63.893	5.170	2.817	1.00 45.68
ATOM	3701	CA	GLY	485	62.692	5.863	3.220	1.00 49.88
ATOM	3702	C	GLY	485	62.216	7.00B	2.337	1.00 53.01
MOTA	3703	O	GLY	485	62.438	7.005	1.117	1.00 50.26
MOTA	3704	N	GLU	486	61.592	8.020	2.949	1.00 56.24
ATOM	3706	CA	GLU	486	61.064	9.183	2.257	1.00 58.07
ATOM	3707	СВ	GLU	486	59.666	8.845	1.682	1.00 55.60
ATOM	3708	C	GLU	486	60.995	10.477	3.088	1.00 59.35
ATOM	3709	0	GLU	486	60.019	11.226	3.000	1.00 61.44
ATOM	3710	N	GLY	487	62.027	10.747	3.879	1.00 59.60
ATOM	3712	CA	GLY	487	62.066	11.964	4.652	1.00 59.75
ATOM	3713	С	GLY	487	61.337	11.959	5.974	1.00 61.44
ATOM	3714	0	GLY	487	61.231	12.979	6.627	1.00 61.96
ATOM	3715	N	ALA	488	60.820	10.800	6.377	1.00 59.69
ATOM	3717	CA	ALA	488	60.134	10.709	7.657	1.00 57.27
ATOM	3718	СВ	ALA	488	59.489	9.337	7.825	1.00 58.05
ATOM	3719	C	ALA	488	61.137	10.970	8.754	1.00 56.28
ATOM	3720	0	ALA	488	60.810	11.446	9.834	1.00 57.31
ATOM	3721	N	PHE	489	62.389	10.630	8.480	1.00 54.40
ATOM	3723	CA	PHE	489	63.462	10.830	9.466	1.00 54.56

ATOM	3724	CB	PHE	489	64.161	9.500	9.770	1.00 49.88
ATOM	3725	CG	PHE	489	63.222	8.454	10.352	1.00 45.21
ATOM	3726	CD1	PHE	489	62.505	7.585	9.516	1.00 43.48
MOTA	3727	CD2	PHE	489	63.017	8.344	11.738	1.00 40.99
ATOM	3728	CE1	PHE	489	61.625	6.653	10.039	1.00 36.69
ATOM	3729	CE2	PHE	489	62.138	7.411	12.257	1.00 35.02
ATOM	3730	CZ	PHE	489	61.433	6.558	11.407	1.00 34.73
ATOM	3731	С	PHE	489	64.456	11.896	8.974	1.00 56.31
ATOM	3732	0	PHE	489	65.372	12.276	9.692	1.00 59.05
MOTA	3733	N	GLY	490	64.285	12.375	7.735	1.00 56.56
ATOM	3735	CA	GLY	490	65.141	13.400	7.143	1.00 55.60
ATOM	3736	С	GLY	·490	65.899	12.778	5.993	1.00 54.79
MOTA	3737	O	GLY	490	65.357	11.854	5.366	1.00 57.10
ATOM	3738	N	GLN	491	67.073	13.304	5.634	1.00 53.44
ATOM	3740	CA	GLN	491	67.829	12.658	4.562	1.00 52.60
ATOM	3741	CB	GLN	491	68.760	13.580	3.777	1.00 53.48
MOTA	3742	CG	GLN	491	69.422	12.818	2.629	1.00 57.19
ATOM	3743	CD	GLN	491	70.046	13.696	1.548	1.00 62.09
ATOM	3744	OE1	GLN	491	70.113	14.893	1.701	1.00 70.26
MOTA	3745	NE2	GLN	491	70.453	13.082	0.441	1.00 62.78
ATOM	3748	C	GLN	491	68.632	11.518	5.165	1.00 49.89
MOTA	3749	0	GLN	491	69.669	11.704	5.805	1.00 49.56
ATOM	3750	N	VAL	492	68.103	10.318	4.984	1.00 47.83
ATOM	3752	CA	VAL	492	68.705	9.093	5.456	1.00 46.38
ATOM	3753	CB	VAL	492	67.760	8.320	6.412	1.00 45.61
ATOM	3754		VAL	492	68 412	7.045	6.932	1.00 46.70
ATOM	3755	CG2	VAL	492	67.361	9.211	7.606	1.00 46.97
ATOM	3756	C	VAL	492	69.004	8.200	4.253	1.00 45.23
ATOM	3757	O	VAL	492	68.181	8.044	3.349	1.00 45.17
ATOM	3758	N	VAL	493	70.210	7.654	4.208	1.00 43.75
ATOM	3760	CA	VAL	493	70.599	6.780	3.109	1.00 44.71
ATOM	3761	CB	VAL	493	71.608	7.471	2.148	1.00 46.20
ATOM	3762		VAL	493	71.159	8.902	1.838	1.00 46.16
ATOM	3763		VAL	493	73.045	7.428	2.706	1.00 42.06
ATOM	3764	С	VAL	493	71.205	5.482	3.624	1.00 44.09
ATOM	3765	0	VAL	493	71.701	5.402	4.745	1.00 43.73
ATOM	3766	N	LEU	494	71.102	4.448	2.809	1.00 43.38
ATOM	3768	CA	LEU	494	71.682	3.158	3.142	1.00 43.29
ATOM	3769	CB	LEU	494	70.988	2.030	2.366	1.00 43.38
ATOM	3770	CG	LEU	494	71.563	0.614	2.431	1.00 39.77
ATOM	3771	CD1		494	71.809	0.201	3.850	1.00 36.38
ATOM	3772	CD2		494	70.600	-0.337	1.760	1.00 42.50
ATOM	3773	C	LEU	494	73.139	3.280	2.725	1.00 42.72
ATOM	3774	0	LEU	494	73.435	3.929	1.720	1.00 43.83
ATOM	3775	N	ALA	495	74.044	2.698	3.499	1.00 40.80
ATOM	3777	CA	ALA	495	75.456	2.785	3.183	1.00 43.80
MOTA	3778	CB	ALA	495	76.059	4.032	3.821	1.00 43.76
ATOM	3779	C	ALA	495	76.171	1.546	3.682	1.00 46.68
ATOM	3780	0	ALA	495	75.668	0.838	4.551	1.00 48.52
ATOM	3781	N	GLU	496	77.330	1.258	3.104	1.00 49.13
ATOM	3783	CA	GLU	496	78.112	0.103	3.519	1.00 49.79
ATOM	3784	CB	GLU	496	78.524	-0.732	2.318	1.00 53.83

MOTA	3785	CG	GLU	496	77.350	-1.224	1.496	1.00 61.33
MOTA	3786	CD	GLU	496	77.623	-2.561	0.862	1.00 64.74
ATOM	3787		GLU	496	76.704	-3.411	0.883	1.00 70.08
MOTA	3788	OE2		496	78.751	-2.760	0.356	1.00 64.12
MOTA	3789	C	GLU	496	79.333	0.601	4.230	1.00 48.46
MOTA	3790	0	GLU	496	80.192	1.236	3.631	1.00 48.79
MOTA	3791	N	ALA	497	79.373	0.375	5.530	1.00 49.25
MOTA	3793	CA	ALA	497	80.503	0.810	6.334	1.00 49.99
MOTA	3794	CB	ALA	497	80.048	1.156	7.732	1.00 48.16
ATOM	3795	С	ALA	497	81.544	-0.301	6.373	1.00 51.53
ATOM	3796	0	ALA	497	81.191	-1.473	6.409	1.00 52.41
MOTA	3797	N	ILE	498	82.821	0.061	6.335	1.00 52.35
ATOM	3799	CA	ILE	498	83.892	-0.928	6.369	100 52.03
MOTA	3800	CB	ILE	498	84.843	-0.797	5.145	1.00 52.83
ATOM	3801	CG2	ILE	498	85.990	-1.795	5.253	1.00 51.43
ATOM	3802	CG1	ILE	498	84.077	-1.006	3.830	1.00 53.85
MOTA	3803	CD1	ILE	498	83.411	0.254	3.271	1.00 55.62
ATOM	3804	C	ILE	498	84.702	-0.802	7.654	1.00 52.74
MOTA	3805	0	ILE	498	85.133	0.293	8.026	1.00 52.14
MOTA	3806	N	GLY	499	84.835	-1.926	8.354	1.00 52.58
MOTA	3808	CA	GLY	499	85.600	-1.974	9.592	1.00 53.03
MOTA	3809	C.	GLY	499	85:165	-1.113	10.771	1.00 53.67
MOTA	3810	0	GLY	499	86.012	-0.544	11.463	1.00 53.99
ATOM	3811	N	LEU	500	83.862	-1.045	11.034	1.00 53.60
ATOM	3813	CA	LEU	500	83.337	-0.245	12.141	1.00 51.00
MOTA	3814	CB	LEU	500	81.841	-0.499	12.317	1.00 49.38
MOTA	3815	CG	LEU	500	80.901	-0.024	11.212	1.00 47.62
MOTA	3816	CD1	LEU	500	79.483	-0.454	11.543	1.00 47.25
MOTA	3817	CD2	LEU	500	80.992	1.486	11.081	1.00 47.38
MOTA	3818	С	LEU	500	84.060	-0.573	13.433	1.00 51.05
ATOM	3819	0	LEU	500	84.396	-1.734	13.670	1.00 53.76
MOTA	3820	N	PRO	505	87.588	-5.968	10.545	1.00 81.81
MOTA	3821	CD	PRO	505	88.588	-6.677	11.357	1.00 81.96
MOTA	3822	CA	PRO	505	88.105	-4.664	10.109	1.00 80.56
MOTA	3823	CB	PRO	505	89.501	-4.622	10.735	1.00 80.75
MOTA	3824	CG	PRO	505	89.868	-6.070	10.860	1.00 82.32
MOTA	3825	С	PRO	505	88.139	-4.477	8.588	1.00 78.53
ATOM	3826	0	PRO	505	88.462	-3.400	8.085	1.00 77.85
ATOM	3827	N	ASN	506	87.792	-5.532	7.865	1.00 77.09
ATOM	3829	CA	ASN	506	87.747	-5.484	6.411	1.00 75.57
ATOM	3830	CB	ASN	506	88.799	-6.415	5.806	1.00 75.80
ATOM	3831	С	ASN	506	86.347	-5.929	6.008	1.00 74.33
MOTA	3832	0	ASN	506	86.044	-6.117	4.826	1.00 73.76
ATOM	3833	N	ARG	507	85.496	-6.092	7.018	1.00 71.72
ATOM	3835	CA	ARG	507	84.120	-6.509	6.820	1.00 69.28
ATOM	3836	CB	ARG	507	83.619	-7.257	8.054	1.00 70.64
ATOM	3837	С	ARG	507	83.258	-5.284	6.605	1.00 65.87
MOTA	3838	0	ARG	507	83.445	-4.262	7.274	1.00 65.40
MOTA	3839	N	VAL	508	82.363	-5.358	5.628	1.00 62.01
MOTA	3841	CA	VAL	508	81.464	-4.248	5.381	1.00 58.41
MOTA	3842	CB	VAL	508	81.043	-4.136	3.915	1.00 57.18
MOTA	3843	CG1	VAL	508	82.251	-3.893	3.046	1.00 61.04

	MOTA	3844	CG2	VAL	508	80.310	-5.383	3.466	1.00 60.74
	ATOM	3845	С	VAL	508	80.257	-4.552	6.246	1.00 56.61
	ATOM	3846	0	VAL	508	79.964	-5.716	6.529	1.00 55.82
	ATOM	3847	N	THR	509	79.572	-3.501	6.665	1.00 54.85
	ATOM	3849	CA	THR	509	78.396	-3.610	7.501	1.00 49.28
	ATOM	3850	CB	THR	509	78.705	-3.144	8.934	1.00 47.98
	MOTA	3851	OG1	THR	509	79.938	-3. 72 7	9.356	1.00 43.39
	MOTA	3853	CG2	THR	509	77.606	-3.565	9.903	1.00 47.57
	MOTA	3854	C	THR	509	77.381	-2.674	6.865	1.00 46.71
	ATOM	3855	0	THR	509	77.675	-1.507	5.625	1.00 48.59
	MOTA	3856	N	LYS	510	76.238	-3.208	6.470	1.00 44.75
	MOTA	3858	CA	LYS	510	75.202	-2.372	5.889	1.00 44.42
-	ATOM	3859	CB ·	LYS	510	74.069	-3.259	5.365	1.00 46.34
	MOTA	3860	CG	LYS	510	73.226	-2.622	4.284	1.00 54.93
	ATOM	3861	CD	LYS	510	73.825	-2.807	2.899	1.00 58.33
	ATOM	3862	CE	LYS	510	73.118	-3.931	2.152	1.00 59.17
	ATOM	3863	NZ	LYS	510	73.317	-5.251	2.813	1.00 56.09
	ATOM	3867	С	LYS	510	74.734	-1. 49 9	7.075	1.00 40.83
	ATOM	3868	O	LYS	510	74.48C	-2.020	8.162	1.00 38.59
	ATOM	3869	N	VAL	511	74.679	.0.183	6.891	1.00 36.28
	ATOM	3871	CA	VAL	511	74.265	0.720	7.957	1.00 31.41
	MOTA	3872	CB	VAL	511	75.480	1.389	8.690	1.00 32.80
	ATOM	3873		VAL	511	76.315	0.346	9.420	1.00 29.97
	ATOM	3874		VAL	511	76.353	2.175	7.706	1.00 30.20
	ATOM ATOM	3875	C	VAL	511	73.408	1 812	7.360	1.00 28.40
	ATOM	3876	0	VAL	511	73.305	1.914	5.147	1.60 27.45
	ATOM	3877	N	ALA	512	72.756	2.598	8.207	1.00 27.30
	ATOM	3879 3880	CA CB	ALA	512	71.953	3.701	7.715	1.00 26.66
	ATOM	3881	CB	ALA ALA	512	70.557	3.640	8.278	1.00 24.24
	ATOM	3882	0	ALA	512 512	72.670	4.965	8.173	1.00 28.52
	ATOM	3883	N	VAL	513	73.140	5.036	9.319	1.00 26.66
	ATOM	3885	CA	VAL	513	72.768 73.442	5.949 7.217	7.275	1.00 29.18
	ATOM	3886	СВ	VAL	513	74.631	7.482	7.569 6.601	1.00 29.65
	ATOM	3887	CG1		513	75.384	8.722	7.015	1.00 28.93
	ATOM	3888	CG2		513	75.570	6.292	6.550	1.00 25.51
	ATOM	3889	C	VAL	513	72.509	8.407	7.476	1.00 29.45 1.00 30.45
	ATOM	3890	0	VAL	513	71.900	8.646	6.431	1.00 30.45
	ATOM	3891	N	LYS	514	72.402	9.143	8.578	1.00 30.13
	ATOM	3893	CA	LYS	514	71.575	10.357	8.654	1.00 33.29
	ATOM	3894	СВ	LYS	514	71.017	10.537	10.068	1.00 38.67
	ATOM	3895	CG	LYS	514	70.074	9.456	10.531	1.00 45.73
	ATOM	3896	CD	LYS	514	69.462	9.860	11.855	1.00 53.93
	ATOM	3897	CE	LYS	514	68.450	8.840	12.337	1.00 63.59
	ATOM	3898	NZ	LYS	514	67.206	8.823	11.517	1.00 71.90
	MOTA	3902	С	LYS	514	72.451	11.568	8.312	1.00 29.45
	ATOM	3903	0	LYS	514	73.584	11.673	8.794	1.00 25.64
	ATOM	3904	N	MET	515	71.918	12.495	7.522	1.00 29.42
	MOTA	3906	CA	MET	515	72.668	13.690	7.119	1.00 30.46
	ATOM	3907	СВ	MET	515	73.464	13.391	5.846	1.00 29.63
	ATOM	3908	CG	MET	515	72.557	13.070	4.665	1.00 32.48
	ATOM	3909	SD	MET	515	73.391	12.475	3.218	1.00 33.06
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ATOM 3910 CE 3.715 1.00 30.26 MET 515 73.734 10.809 MOTA 3911 C 6.848 MET 515 71.700 14.839 1.00 30.75 MOTA 3912 0 MET 70.478 14.654 6.867 515 1.00 33.07 MOTA 3913 N LEU 516 72.238 16.027 6.608 1.00 30.32 MOTA 3915 CA LEU 17.194 516 71.414 6.304 1.00 30.21 3916 MOTA CB LEU 516 72.112 18.487 6.748 1.00 26.54 MOTA 3917 CG LEU 516 72.452 18.668 8.227 1.00 23.97 MOTA 3918 CD1 73.345 19.858 1.00 24.27 LEU 516 8.412 71.198 MOTA 3919 CD2 LEU 516 18.850 9.023 1.00 21.46 **ATOM** 3920 C LEU 516 71.197 17.265 4.800 1.00 33.44 MOTA 3921 0 LEU 516 72.016 16.784 4.015 1.00 34.50 **ATOM** 3922 N LYS 517 70.082 17.863 4.400 1.00 36.36 **MOTA** 3924 CA . LYS .517.. 69.783 18.048 2.993 1.00 34.58 3925 ATOM CB LYS 517 68.281 18.255 2.784 1.00 38.96 **ATOM** 3926 CG LYS 517 67.409 17.155 3.380 1.00 44.34 3927 **ATOM** CD LYS 517 66.128 16.920 2.572 1.00 52.11 3928 **ATOM** CE LYS 517 65.138 18.083 2.637 1.00 58.29 **ATOM** 3929 NZ LYS 517 63.915 17.833 1.786 1.00 60.90 **ATOM** 3933 С LYS 517 70.567 19.304 2.597 1.00 33.51 **ATOM** 3934 0 LYS 20.064 517 71.024 3.460 1.CO 30.34 MOTA 3935 N SER 518 70.701 19.539 1.296 1.00 34.39 **ATOM** 3937 CA SER 20.693 0.788 518 71.444 1.00 35.84 ATOM 3938 CB SER 71.537 -0.731 518 20.618 1.00 33.66 MOTA 3939 OG SER 518 70.282 20.258 -1.266 1.00 38.73 **ATOM** 3941 С SER 518 70.879 22.045 1.198 1.00 36.91 MOTA 3942 Ú SER 518 71.591 23.050 1.205 1.00 37.32 MOTA 3943 N ASP 519 59.598 22.069 1.538 1.00 37.88 **ATOM** 3945 CA ASP 519 68.945 23.313 1.936 1.00 38.83 MOTA 3946 CB ASP 519 67.517 23.364 1.375 1 00 42.23 **ATOM** 3947 CG ASP 1.775 519 66.669 22.151 1.00 48.87 **ATOM** 3948 OD1 ASP 1.00 49.21 519 67.070 21.380 2.681 ATOM 3949 OD2 ASP 519 65.582 21.972 1.181 1.00 54.93 **MOTA** 3950 C ASP 519 68.916 23.537 3.443 1.00 38.06 **ATOM** 3951 0 ASP 519 68.246 24.451 3.916 1.00 39.38 MOTA 3952 N ALA 520 69.622 22.692 4.191 1.00 36.24 MOTA 3954 CA ALA 520 69.631 22.795 5.648 1.00 34.69 **ATOM** 3955 CB ALA 520 70.359 21.613 6.259 1.00 35.68 MOTA 3956 C ALA 520 70.213 24.087 1.00 33.54 6.173 ATOM 3957 0 ALA 520 71.039 24.718 5.522 1.00 34.83 **ATOM** 3958 THR N 521 69.815 24.452 7.384 1.00 34.45 MOTA 3960 CA THR 521 70.315 25.668 8.001 1.00 36.51 **MOTA** 3961 CB THR 521 69.148 26.592 8.493 1.00 39.14 **ATOM** 3962 OG1 THR 521 68.529 26.031 9.659 1.00 41.61 **ATOM** 3964 CG2 THR 521 68.081 26.750 7.409 1.00 40.14 3965 **ATOM** С THR 71.228 521 25.303 9.170 1.00 36.35 **ATOM** 3966 0 THR 521 71.376 24.125 9.510 1.00 32,23 MOTA 3967 N GLU 522 71.868 26.310 9.756 1.00 39.33 MOTA 3969 CA **GLU** 522 72.747 26.092 10.890 1.00 44.59 **ATOM** 3970 CB GLU 522 73.364 11.335 1.00 51.80 27.424 **ATOM** 3971 CG GLU 522 74.463 27.311 12.418 1.00 64.10 MOTA 75.811 3972 CD GLU 522 26.815 11.886 1.00 69.12 ATOM 3973 OE1 GLU 522 76.784 27.605 11.869 1.00 69.26

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ATOM	3974	OE2	GLU	522	75.900	25.629	11.502	1.00 73.62
ATOM	3975	С	GLU	522	71.953	25.447	12.042	1.00 44.53
ATOM	3976	0	GLU	522	72.482	24.617	12.786	1.00 44.95
ATOM	3977	N	LYS	523	70.679	25.814	12.167	1.00 42.99
ATOM	3979	CA	LYS	523	69.826	25.264	13.216	1.00 42.17
ATOM	3980	CB	LYS	523	68.519	26.053	13.329	1.00 45.99
MOTA	3981	CG	LYS	523	67.583	25.582	14.433	1.00 48.74
ATOM	3982	CD	LYS	523	66.296	25.027	13.832	1.00 57.24
ATOM	3983	CE	LYS	523	65.405	24.383	14.884	1.00 60.31
ATOM	3984	NZ	LYS	523	64.309	23.586	14.247	1.00 65.17
ATOM	3988	С	LYS	523	69.563	23.793	12.935	1.00 39.03
MOTA	3989	Ο.	LYS	523	69.581	22.973	13.850	1.00 40.65
ATOM	3990	N	ASP	524	··69 . 331	23 457	11.672	1.00 34.91
ATOM	3992	C'A	ASP	524	69.122	22.068	11.294	1.00 33.12
ATOM	3993	CB	ASP	524	68.876	21.942	9.790	1.00 34.84
ATOM	3994	CG	ASP	524	67.482	22.352	9.389	1.00 36.47
MOTA	3995	OD1	ASP	524	66.552	22.193	10.204	1.00 41.59
ATOM	3996	OD2	ASP	524	67.307	22.815	8.248	1.00 38.19
ATOM	3997	С	ASP	524	70.383	21.284	11.653	1.00 33.94
ATOM	3998	0	ASP	524	70.301	20.154	12.139	1.00 37.40
ATOM	3999	N	LEU	525	71.554	21.869	11.404	1.00 32.39
ATOM	4001	CA	LEU	525	72.799	21.186	11.729	1.00 31.50
ATOM	4002	CB	LEU	525	74.018	21.998	11.278	1.00 29.05
ATOM	4003	CG	LEU	525	75.363	21.375	11.680	1.00 28.38
ATOM	4004		LEU	525	75.521	19.990	11.065	1.00 27.27
ATOM	4005		LEU	525	76:519	32.283	11.295	1 00 26.26
ATOM	4005	C	LEU	525	72.848	20.941	13.231	1.00 30.27
ATOM	4007	O	LEU	525	73.104	19.828	13.675	1.00 33.58
ATOM	4008	N	SER	526	72.563	21.982	14.000	1.00 29.63
ATOM	4010	CA	SER	526	72.544	21.914	15.459	1.00 30.26
ATOM	4011	CB	SER	526	72.046	23.251	16.013	1.00 32.03
ATOM	4012	OG	SER	526	71.923	23.199	17.417	1.00 37.02
ATOM	4014	C	SER	526	71.640	20.796	15.980	1.00 29.72
ATOM	4015	0	SER	526	71.924	20.162	16.998	1.00 27.54
ATOM	4016	N	ASP	527	70.525	20.588	15.291	1.00 28.97
ATOM	4018	CA	ASP	527	69.581	19.556	15.664	1.00 29.28
ATOM	4019	CB	ASP	527	68.289	19.710	14.855	1.00 29.08
ATOM	4020	CG	ASP	527	67.497	20.977	15.225	1.00 30.05
ATOM	4021	OD1		527	67.750	21.597	16.292	1.00 24.32
ATOM	4022	OD2		527	66.591	21.335	14.436	1.00 34.69
ATOM	4023	C	ASP	527	70.175	18.164	15.436	1.00 30.65
ATOM	4024	0	ASP	527	70.115	17.297	16.312	1.00 30.12
ATOM	4025	N	LEU	528	70.769	17.958	14.265	1.00 30.50
ATOM	4027	CA	LEU	528	71.358	16.669	13.946	1.00 29.54
ATOM	4028	CB	LEU	528	71.850	16.647	12.487	1.00 26.03
ATOM	4029	CG	LEU	528	72.409	15.320	11.942	1.00 24.26
ATOM	4030	CD1		528	71.466	14.142	12.259	1.00 21.51
ATOM	4031	CD2		528	72.644	15.437	10.450	1.00 15.05
ATOM	4032	C	LEU	528	72.494	16.342	14.933	1.00 30.51
ATOM	4033	0	LEU	528	72.641	15.192	15.354	1.00 29.79
ATOM	4034	N	ILE	529	73.281	17.351	15.305	1.00 30.86
ATOM	4036	CA	ILE	529	74.367	17.138	16.253	1.00 28.41

ATOM	4037	CB	ILE	529	75.266	18.349	16.406	1.00 24.75	
ATOM	4038	CG2	ILE	529	76.355	18.064	17.432	1.00 25.51	
ATOM	4039	CG1	ILE	529	75.901	18.710	15.084	1.00 17.82	
ATOM	4040	CD1	ILE	529	76.912	19.806	15.251	1.00 18.14	
ATOM	4041	C	ILE	529	73.821	16.813	17.641	1.00 30.17	
ATOM	4042	0	ILE	529	74.286	15.873	18.285	1.00 30.11	
MOTA	4043	N	SER	530	72.836	17.574	18.101	1.00 30.29	
ATOM	4045	CA	SER	530	72.271	17.310	19.418	1.00 33.14	
ATOM	4046	CB	SER	530	71.158	18.293	19.735	1.00 36.09	
MOTA	4047	OG	SER	530	76.224	18.323	18.670	1.00 49.01	
ATOM	4049	C	SER	530	71.740	15.881	19.479	1.00 33.80	
MOTA	4050	Û	SER	530	71.896	15.190	20.492	1.00 37.06	
MOTA	4051	N	GLU	531	71.156	15.413	18.378	1.00 30.13	
ATOM	4053	CA	GLU	531	70.629	14.065	18.351	1.00 29.18	
ATOM	4054	CB	GLU	531	69.822	13.801	17.087	1.00 32.42	
ATOM	4055	CG	GLU	531	69.253	12.394	17.058	1.00 33.35	
MOTA	4056	CD	GLU	531	68:354	12.131	15.883	1.00 34.76	
MOTA	4057	OEl	GLU	531	67.481	11.249	16.002	1.00 40.42	
ATOM	4058	OE2	GLU	531	68.516	12:793	14.847	1.00 35.88	
ATOM	4059	C	GLU	531	71.734	13.025	18.488	1.00 28.27	
ATOM	4060	0	GLU	531	71.569	12.032	19.192	1.00 26.75	
ATOM	4061	N	MET	532	72.842	13.235	17.786	1.00 27.80	
ATOM	4063	CA	MET	532	73.976	12.320	17.835	1.00 27.82	
MOTA	4064	CB	MET	532	75.080	12.813	16.890	1.00 29.43	
ATOM	4065	CG	MET	532 .	76.461	12.225	17.138	1.00 24.34	
ATOM	4066	SD	MET	532	77.641	12.702	15.840	1.00 27.83	
ATOM	4067	CE	MET	532	77.791.	14.452	16.193	1.00 21.90	
ATOM	4068	С	MET	532	74.499	12.272	19.260	1.00 29.53	
ATOM	4069	0	MET	532	74.742	11.197	19.809	1.00 30.14	
ATOM	4070	N	GLU	533	74.610	13.445	19.871	1.00 30.25	
ATOM	4072	CA	GLU	533	75.109	13.570	21.233	1.00 31.95	
ATOM	4073	CB	GLU	533	75.300	15.039	21.594	1.00 32.55	
MOTA	4074	CG	GLU	533	76.391	15.724	20.765	1.00 35.71	
MOTA	4075	CD	GLU	533	77.766	15.087	20.951	1.00 36.71	
MOTA	4076		GLU	533	78.297	15.136	22.084	1.00 40.19	
ATOM	4077	OE2	GLU	533	78.322	14.555	19.969	1.00 33.99	
ATOM	4078	C	GLU	533	74.185	12.886	22.225	1.00 33.06	
ATOM	4079	0	GLU	533	74.642	12.197	23.147	1.00 33.49	
MOTA	4080	N	MET	534	72.883	13.052	22.025	1.00 33.12	
ATOM	4082	CA	MET	534	71.913	12.432	22.900	1.00 32.48	
ATOM	4083	CB	MET	534	70.484	12.859	22.533	1.00 30.60	
ATOM	4084	CG	MET	534	69.591	12.915	23.791	0.50 28.70	PRT1
ATOM	4085	SD	MET	534	67.787	12.849	23.608	0.50 27.55	PRT1
MOTA	4086	CE	MET	534	67.409	14.560	23.291	0.50 26.84	PRT1
MOTA	4087	С	MET	534	72.102	10.908	22.785	1.00 31.10	
ATOM	4088	Ò	MET	534	72.258	10.224	23.791	1.00 32.80	
ATOM	4089	N	MET	535	72.194	10.394	21.563	1.00 30.50	
MOTA	4091	CA	MET	535	72.399	8.961	21.368	1.00 29.25	
ATOM	4092	CB	MET	535	72.577	8.623	19.884	1.00 28.10	
ATOM	4093	CG	MET	535	71.337	8.876	19.042	1.00 27.48	
ATOM	4094	SD	MET	535	71.377	7.980	17.502	1.00 26.94	
ATOM	4095	CE	MET	535	71.346	9.275	16.310	1.00 33.72	

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ATOM	4096	С	MET	5 35	73.621	8.514	22.155	1.00	29.29
ATOM	4097	0	MET	535	73.640	7.412	22.710	1.00	29.06
MOTA	4098	N	LYS	536	74.644	9.367	22.185	1.00	31.75
ATOM	4100	CA	LYS	536	75.869	9.073	22.930	1.00	33.24
MOTA	4101	CB	LYS	536	76.950	10.108	22.628	1.00	31.29
MOTA	4102	CG	LYS	536	77.602	10.007	21.258	1.00	31.09
ATOM	4103	CD	LYS	536	78.570	11.154	21.103	1.00	28.76
MOTA	4104	CE	LYS	536	79.219	11.220	19.755		26.70
ATOM	4105	NZ	LYS	536	80.059	12.461	19.742		27.38
ATOM	4109	C	LYS	536	75.630	9.014	24.451		35.30
ATOM	4110	O	LYS	536	76.201	8.172	25.137		35.61
MOTA	4111	N	MET	537	74.788	9.902	24.972		35.67
MOTA	4113	CA	MET	537	74.517	9.908	26.408	1.00	38.27
MOTA	4114	CB	MET	537	73.858	11.221	26.844		43.86
MOTA	4115	CG	MET	537	74.801	12.420	26.884		55.46
ATOM	4116	SD	MET	537	76.189	12.272	28.062		63.44
ATOM	4117	CE	MET	537	75.383	12.822	29.591		62.14
ATOM	4118	C	MET	537	73.657	8.734	26.845		37.10
ATOM	4119	0	MET	537	73.855	8.188	27.920	1.00	39.26
ATOM	4120	N	ILE	538	72., 723	8.320	26.003	1.00	34.96
ATOM	4122	CA	ILE	538	71.819	7.219	26.320		32.78
ATOM	4123	CB	ILE	538	70.618	7.202	25.342		32.48
ATOM	4124	CG2	ILE	538	69.782	5.943	25.537		32.27
ATOM	4125	CG1	ILE	538	69.756	8.449	25.538	1.00	31.77
ATOM	4126	CD1	ILE	538	68.746	8.651	24.409	1.00	34.25
MOTA	4127	C	ILE	538	72.456	5.823	26.365	1.00	30.54
ATOM	4128	0	ILE	538	72.146	5.039	27.250	1.00	33.37
ATOM	4129	N	GLY	539	73.293	5.481	25.399	1.00	27.09
MOTA	4131	CA	GLY	539	73.892	4.162	25.419	1.00	28.72
ATOM	4132	С	GLY	539	73.173	3.135	24.552	1.00	31.16
MOTA	4133	0	GLY	539	72.069	3.379	24.060	1.00	32.94
MOTA	4134	N	LYS	540	73.808	1.981	24.370	1.00	31.68
MOTA	4136	CA	LYS	540	73.264	0.912	23.537	1.00	34.64
MOTA	4137	CB	LYS	540	74.399	0.032	23.029	1.00	33.47
ATOM	4138	CG	LYS	540	75.331	0.730	22.095	1.00	39.67
ATOM	4139	CD	LYS	540	76.396	-0.209	21.573	1.00	41.48
ATOM	4140	CE	LYS	540	77.228	0.475	20.501	1.00	48.72
ATOM	4141	NZ	LYS	540	76.442	0.800	19.254	1.00	54.86
ATOM	4145	C	LYS	540	72.206	-0.010	24.143	1.00	36.68
ATOM	4146	0	LYS	540	72.276	-0.370	25.324	1.00	
MOTA	4147	N	HIS	541	71.233	-0.396	23.319	1.00	35.61
MOTA	4149	CA	HIS	541	70.190	-1.335	23.711	1.00	34.24
ATOM	4150	CB	HIS	541	69.074	-0.702	24.526	1.00	33.44
ATOM	4151	CG	HIS	541	68.118	-1.711	25.083	1.00	34.60
MOTA	4152		HIS	541	68.059	-2.310	26.292	1.00	33.77
ATOM	4153		HIS	541	67.143	-2.316	24.309	1.00	34.19
MOTA	4155		HIS	541		-3.248	25.020	1.00	36.87
ATOM	4156		HIS	541	67.074	-3.272	26.228	1.00	34.05
ATOM	4158	C	HIS	541	69.624	-2.023	22.474	1.00	
ATOM	4159	0	HIS	541	69.342	-1.378	21.457	1.00	38.40
MOTA	4160	N	LYS	542	69.407	-3.331	22.586	1.00	36.42
MOTA	4162	CA	LYS	542	68.923	-4.155	21.469	1.00	

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MOTA	4163	CB	LYS	542	68.680	-5.602	21.915	1.00 34.24
MOTA	4164	C	LYS	542	67.674	-3.646	20.802	1.00 32.40
ATOM	4165	0	LYS	542	67.507	-3.822	19.612	1.00 32.37
MOTA	4166	N	ASN	543	66.785	-3.046	21.580	1.00 32.12
ATOM	4168	CA	ASN	543	65.541	-2.561	21.015	1.00 33.01
ATOM	4169	CB	ASN	543	64.361	-3.081	21.842	1.00 34.26
MOTA	4170	CG	ASN	543	64.365	-4.597	21.979	1.00 32.20
ATOM	4171	OD1	ASN	543	64.633	-5.128	23.050	1.00 32.23
MOTA	4172		ASN	543	64.077	-5.292	20.904	1.00 30.50
ATOM	4175	C	ASN	543	65.424	-1.050	20.719	1.00 32.21
ATOM	4176	O	ASN	543	64.326	-0.481	20.765	1.00 31.13
ATOM	4177	N	ILE	544	66.556	-0.419	20.397	1.00 30.52
ATOM	41.79	CA	ILE	544	66.611	1.002	20028	1.00 29.01
MOTA	4180	CB	ILE	544	67.040	1.962	21.208	1.00 25.83
ATOM	4181	CG2	ILE	544	66.244	1.682	22.467	1.00 24.46
ATOM	4182	CG1	ILE	544	68.532	1.848	21.522	1.00 27.54
ATOM	4183	CD1	ILE	544	69.008	2.839	22.581	1.00 22.70
MOTA	4184	С	ILE	544	67.617	1.118	18.870	1.00 23.49
ATOM	4185	0	ILE	544	68.410	0.194	18.€33	1.00 27.26
MOTA.	4186	N	ILE	545	67.504	2.184	18.078	1.00 26.74
ATOM	4188	CA	ILE	545	68.453	2.396	16.992	1.00 27.06
MOTA	4189	CB	ILE	545	67.913	3.350	15.921	1.00 23.64
ATOM	4190	CG2		545	69.027	3.727	14.955	1.00 23.96
ATOM	4191		ILE	545	66.754	2.692	15.167	1.00 23.13
MOTA	4192		ILE	545	67.152	1.481	14.339	1.00 20.61
ATOM	4193	С	ILE	545	69.720	2.968	17.633	1.00 26.93
ATOM	4194	Ç	ILE	545	69.719	4.075	18.160	1.00 28.63
ATOM	4195	N	ASN	546	70.800	2.200	17.560	1.00 28.53
MOTA	4197	CA	ASN	546	72.075	2.567	18.161	1.00 29.39
ATOM	4198	CB	ASN	546	72.752	1.308	18.718	1.00 29.14
ATOM	4199	CG	ASN	546	71.908	0.613	19.772	1.00 30.21
ATOM	4200		ASN	546	71.804	1.088	20.899	1.00 30.74
ATOM	4201		ASN	546	71.290	-0.505	19.406	1.00 30.79
ATOM	4204	C	ASN	546	73.034	3.303	17.238	1.00 30.78
MOTA	4205	0	ASN	546	73.011	3.126	16.015	1.00 33.04
ATOM	4206	N	LEU	547	73.866	4.151	17.837	1.00 31.07
MOTA	4208	CA	LEU	547	74.880	4.904	17.101	1.00 31.37
MOTA	4209	CB	LEU	547	75.284	6.165	17.875	1.00 27.32
ATOM	4210	CG	LEU	547	76.413	7.032	17.297	1.00 24.17
MOTA	4211		LEU	547	75.953	7.768	16.069	1.00 18.06
ATOM ATOM	4212		LEU	547	76.864	8.014	18.348	1.00 22.50
ATOM	4213	C	LEU	547	76.107	3.999	16.861	1.00 33.38
	4214	0	LEU	547	76.610	3.343	17.789	1.00 33.58
ATOM ATOM	4215	N	LEU	548	76.543	3.919	15.607	1.00 32.72
	4217	CA	LEU	548	77.694	3.104	15.259	1.00 31.50
ATOM ATOM	4218	CB	LEU	548 548	77.388	2.244	14.029	1.00 26.30
	4219	CG	LEU	548	76.148	1.341	14.158	1.00 25.93
ATOM	4220		LEU	548	76.034	0.513	12.906	1.00 28.37
ATOM	4221		LEU	548	76.196	0.436	15.394	1.00 15.84
ATOM	4222	C	LEU	548	78.941	3.965	15.030	1.00 33.69
ATOM	4223	0	LEU	548	80.063	3.488	15.167	1.00 37.41
ATOM	4224	И	GLY	549	78.746	5.229	14.675	1.00 34.10

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ATOM	4226	CA	GLY	549	79.871	6.116	14.454	1.00 31.50
ATOM	4227	С	GLY	549	79.425	7.429	13.839	1.00 31.11
ATOM	4228	0	GLY	549	78.221	7.686	13.700	1.00 30.15
ATOM	4229	N	ALA	550	80.388	8.268	13.474	1.00 31.02
MOTA	4231	CA	ALA	550	80.074	9.540	12.850	1.00 29.00
MOTA	4232	CB	ALA	550	79.537	10.526	13.899	1.00 27.87
ATOM	4233	C	ALA	550	81.257	10.149	12.102	1.00 27.66
MOTA	4234	0	ALA	550	82.422	9.942	12.474	1.00 25.24
MOTA	4235	N	CYS	551	80.944	10.810	10.984	1.00 27.61
ATOM	4237	CA	CYS	551	81.924	11.540	10.170	1.00 25.02
MOTA	4238	CB	CYS	551	81.754	11.237	8.680	1.00 22.41
ATOM	4239	SG	CYS	551	82.155	⁵ 9.553	8.187	1.00 27.24
ATOM	4240	C .	CYS	551	81.583	13.009	10.447	1-00-24-31
ATOM	4241	O	CYS	551	80.569	13.525	9.958	1.00 23.55
MOTA	4242	N	THR	552	82.367	13.657	11.303	1.00 23.22
MOTA	4244	CA	THR	552	82.110	15.046	11.664	1.00 25.73
MOTA	4245	CB	THR	552	82.138	15.215	13.202	1.00 26.50
MOTA	4246	OG1	THR	552	B3.479	15.031	13.664	1.00 26.31
ATOM	4248	CG2	THR	552	81.257	14.171	13.886	1.00 26.64
ATOM	4249	C	THR	552	83.134	16.014	11.090	1.00 27.93
ATOM	4250	C	THR	552	82.894	17216	11.005	1.00 28.35
ATOM	4251	N	GLN	553	84.264	15.473	10.663	1.00 30.26
ATOM	4253	CA	GLN	553	85.355	16.288	10.153	1.00 29.27
MOTA	4254	CB	GI.N	553	86.669	15.768	10.763	J. 00 29,54
ATOM	4255	CG	GLN	553	86.653	15.655	12.288	1.00 28.00
ATOM	4256	CD	GLN	553	86.534	17.007	12.981	1.00 26.86
ATOM	4257	OE1	GLN	553	87.440	17.821	12.902	1.00 30.85
ATOM	4258	NE2	GLN	553	85.421	17.239	13.676	1.00 23.89
ATOM	4261	С	GLN	553	85.475	16.316	8.634	1.00 28.30
ATOM	4262	0	GLN	553	85.221	15.313	7.967	1.00 31.00
ATOM	4263	N	ASP	554	85.860	17.480	8.119	1.00 26.89
ATOM	4265	CA	ASP	554	86.070	17.725	6.695	1.00 27.85
ATOM	4266	CB	ASP	554	87.370	17.081	6.257	1.00 33.44
ATOM	4267	CG	ASP	554	88.534	17.564	7.060	1.00 37.63
ATOM	4268		ASP	554	89.038	18.664	6.763	1.00 42.66
ATOM	4269		ASP	554	88.929	16.843	8.000	1.90 35.80
ATOM	4270	C	ASP	554	84.976	17.341	5.715	1.00 28.04
ATOM ATOM	4271	0	ASP	554	85.193	16.518	4.826	1.00 31.06
ATOM ATOM	4272	N	GLY	555	83.824	17.981	5.842	1.00 28.26
ATOM ATOM	4274	CA	GLY	555	82.720	17.694	4.949	1.00 25.89
ATOM ATOM	4275 4276	C	GLY	555	81.438	17.567	5.734	1.00 23.07
ATOM ATOM		0	GLY	555	81.423	17.795	6.941	1.00 20.20
ATOM ATOM	4277	N	PRO	556	80.338	17.185	5.076	1.00 22.81
	4278	CD	PRO	556	80.280	16.750	3.679	1.00 22.33
ATOM ATOM	4279	CA	PRO	556	79.039	17.032	5.733	1.00 23.99
ATOM ATOM	4280	CB	PRO	556 556	78.154	16.499	4.612	1.00 22.41
ATOM ATOM	4281 4282	CG C	PRO	556	79.144	15.801	3.698	1.00 24.36
ATOM ATOM			PRO	556	79.080	16.066	6.911	1.00 26.98
ATOM ATOM	4283	0	PRO	556 553	79.854	15.111	6.934	1.00 28.57
ATOM ATOM	4284	N	LEU	557	78.237	16.325	7.896	1.00 29.25
	4286	CA	LEU	557	78.168	15.471	9.070	1.00 30.83
ATOM	4287	CB	LEU	557	7 7.550	16.225	10.251	1.00 33.20

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ATOM 4288 CG LEU 557 77.109 15.416 11.475 1.00 30.01 **ATOM** 4289 CD1 LEU 14.793 12.174 557 78.304 1.00 29.05 **ATOM** 4290 CD2 LEU 557 76.365 16.341 12.407 1.00 29.20 14.238 8.780 **ATOM** 4291 C LEU 557 77.324 1.00 30.33 **ATOM** 4292 0 14.343 8.330 LEU 557 76.175 1.00 27.66 MOTA 4293 13.071 9.002 N TYR 558 77.913 1.00 30.68 **ATOM** 4295 77.214 11.823 CA TYR 558 8.812 1.00 29.26 MOTA 4296 CB TYR 558 77.978 10.933 7.840 1.00 30.99 **ATOM** 4297 11.481 CG TYR 558 78.066 6.430 1.00 35.01 **ATOM** 4298 CD1 TYR 558 79.108 11.109 5.592 1.00 36.17 **ATOM** 4299 CE1 TYR 558 79.198 11.600 4.296 1.00 41.40 **ATOM** 4300 CD2 TYR 558 77.109 12.368 5.941 1.00 36.44 ATOM 4301 -CE2-TYR -558 77.188 12.871 4.648 1.00 40.96 **ATOM** 12.484 3.825 1.00 43.59 4302 CZTYR 558 78.237 MOTA 4303 ОН TYR 558 78.298 12.965 2.525 1.00 42.91 TYR **ATOM** 4305 C 558 77.081 11.125 10.164 1.00 28.18 MOTA 4306 10.835 C TYR 558 78.077 10.855 1.00 28.06 **ATOM** 4307 N VAL 559 75.842 10.879 10.574 1.00 26.72 ATOM 4309 VAL CA 559 75.548 10.175 11.821 1.00 26.72 **ATOM** 4310 CB VAL 559 74.326 10.813 12.552 1.00 28.03 ATOM 4311 CG1 VAL 559 73.915 9.992 13.771 1.00 29.85 MOTA 4312 CG2 VAL 559 74.655 12.236 12.982 1.00 29.37 MOTA 4313 VAL 8.723 1.00 25.58 C 559 75.238 11.443 MOTA 4314 0 VAL 559 74.131 8.402 10.988 1.00 25.73 ATOM 4315 ILE 7.851 N 560 76.214 11.642 1.00 24.35 MOTA 4317 CA ILE 76.061 6.448 11.281 560 1.00 26.64 MOTA 4318 CB ILE 560 77.441 5.781 11.002 1.00 26.53 MOTA 4319 CG2 ILE 560 77.252 4.359 10.465 1.00 27.80 MOTA 4320 CG1 ILE 78.254 6.620 560 10.004 1.00 24.69 ATOM 4321 CD1 ILE 73.671 6.112 9.763 560 1.00 17.05 **ATOM** 4322 ILE 75.312 5.633 C 560 12.339 1.00 27.95 MOTA 75.777 4323 ILE 5.493 13.479 0 560 1.00 25.16 ATOM 4324 VAL N 561 74.163 5.084 11.951 1.00 27.43 MOTA 4326 CA VAL 561 73.352 4.265 12.847 1.00 27.69 MOTA 4327 CB VAL 561 72.048 5.000 13.251 1.00 25.08 MOTA 4328 CG1 VAL 72.367 6.302 561 13.936 1.00 19.97 MOTA 4329 CG2 VAL 561 71.186 5.250 12.033 1.00 25.55 MOTA 4330 C VAL 561 73.031 2.896 12.202 1.00 30.21 MOTA 4331 0 VAL 561 73.404 2.623 11.045 1.00 32.04 GLU **ATOM** 4332 N 562 72.306 2.062 12.944 1.00 28.88 MOTA GLU 4334 CA 562 71.940 0.714 12.509 1.00 27.69 MOTA 4335 CB GLU 562 71.448 -0.081 13.712 1.00 26.79 **ATOM** 4336 CG GLU 72.387 0.001 1.00 28.13 562 14.873 **ATOM** 4337 CD GLU 562 72.012 -0.916 16.003 1.00 31.86 **ATOM** 4338 OE1 GLU 72.772 -1.876 562 16.255 1.00 33.17 **ATOM** OE2 GLU 4339 70.974 562 -0.654 16.639 1.00 35.50 ATOM 4340 С GLU 562 70.898 0.636 11.405 1.00 27.34 **ATOM** 4341 0 GLU 562 69.990 1.453 11.358 1.00 29.72 ATOM 4342 71.002 N TYR 563 -0.392 1.00 28.07 10.568 ATOM CA -0.626 4344 TYR 563 70.080 9.455 1.00 32.50 **ATOM** 4345 CB TYR 563 70.848 -1.2368.269 1.00 28.32 ATOM 4346 CG TYR 563 70.042 -1.4277.007 1.00 26.56

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ATOM 4347 CD1 TYR 563 69.338 -0.378 6.448 1.00 30.49 ATOM 4348 CE1 TYR 563 68.620 -0.536 5.258 1.00 32.83 ATOM 4349 CD2 TYR 563 70.011 -2.652 6.350 1.00 29.07 ATOM 4350 CE2 TYR 563 69.300 -2.821 5.151 1.00 30.70 **ATOM** 4351 CZ TYR 563 68.605 4.619 -1.755 1.00 33.54 ATOM 4352 OH TYR 563 67.876 -1.919 3.460 1.00 40.20 ATOM 4354 C TYR 563 68.930 -1.564 9.878 1.00 36.30 ATOM 4355 0 TYR 563 69.151 -2.569 10.562 1.00 36.17 **ATOM** 4356 N ALA 564 67.711 -1.234 9.454 1.00 39.60 **ATOM** 4358 CA ALA 564 66.529 9.750 -2.025 1.00 38.93 **ATOM** 4359 CB ALA 564 65.557 -1.207 10.570 1.00 40.23 ATOM 4360 °C ALA 564 65.919 -2.360 8.394 1.00 41.61 MOTA 4361 0 ALA · 564 .. 64.958 -1.736 7.977 1.00 45.88 ATOM 4362 N 7.745 SER 565 66.455 -3.387 1.00 41.15 **ATOM** 4364 CA SER 565 66.018 -3.806 6.421 1.00 40.40 **ATOM** 4365 CB SER 565 66.673 -5.134 6.070 1.00 40.15 ATOM 4366 OG SER 565 66.646 -6.012 7.175 1.00 33.93 MOTA 4368 С SER 565 64.530 1.00 40.31 ~3.932 6.164 MOTA 4369 0 SER 565 64.097 ~3.823 5.025 1.00 45.43 MOTA 4370 N LYS 566 63.743 -4.183 7.197 1.00 39.63 MOTA 4372 CA LYS 566 62'.312 -4.341 6.992 1.00 38.01 ATOM 4373 CB LYS 566 61.807 -5.541 7.783 1.00 38.35 MOTA 4374 CG LYS 566 62.468 -6.828 7.308 1.00 38.21 MOTA 4375 CD LYS 566 62.161 -8.004 8.208 1.00 38.79 ATOM 4376 CE LYS 566 62.734 .-9.277 7.621 1.00 38.76 **ATOM** 4377 NZ LYS 566 62.692 -10.400 8.598 1.00 42.40 .ATOM 4381 С LYS 566 61.488 -3.079 7.249 1.00 37.28 MOTA 4382 Ο LYS 566 60.265 1.00 39.48 -3.132 7.415 **ATOM** 4383 N GLY 567 62.166 -1.936 7.237 1.00 34.31 MOTA 4385 CA GLY 567 61.497 -0.666 7.428 1.00 32.82 MOTA 4386 C GLY 567 60.810 -0.473 8.761 1.00 31.33 ATOM 4387 O GLY 567 61.251 -1.012 9.778 1.00 29.23 **ATOM** 4388 N ASN 568 59.722 0.294 8.754 1.00 29.92 **ATOM** 4390 CA ASN 56.8 58.999 9.974 0.569 1.00 31.05 **ATOM** 4391 CB ASN 568 58.414 9.991 1.991 1.00 31.23 ATOM 4392 CG ASN 568 57.201 9.087 2.157 1.00 34.16 MOTA 4393 OD1 ASN 568 56.095 9.385 1.685 1.00 37.22 ATOM 4394 ND2 ASN 568 57.394 2.877 7.999 1.00 35.13 **ATOM** 4397 С ASN 568 57.950 -0.486 10.235 1.00 31.60 **ATOM** 4398 0 ASN 568 57.535 1.00 31.76 -1.205 9.324 MOTA 4399 N LEU 569 57.517 -0.548 11.490 1.00 34.63 MOTA 4401 CA LEU 569 56.540 -1.511 11.979 1.00 35.49 **ATOM** 4402 CB LEU 569 56.456 13.500 -1.408 1.00 36.13 **ATOM** 4403 CG LEU 569 55.509 -2.363 14.210 1.00 34.78 MOTA 4404 CD1 LEU 569 56.010 14.034 -3.804 1.00 35.01 **ATOM** 4405 CD2 LEU 569 55.425 -1.971 15.664 1.00 31.13 ATOM 4406 C LEU 569 55.141 -1.420 11.382 1.00 37.34 MOTA 4407 LEU 0 569 54.518 -2.447 11.141 1.00 41.49 MOTA 4408 N ARG 570 54.636 -0.213 11.162 1.00 37.19 MOTA 4410 CA ARG 570 53.299 -0.063 10.591 1.00 39.79 **ATOM** 4411 CB ARG 570 52.979 1.403 10.331 1.00 39.48 ATOM 4412 CG ARG 570 51.558 1.638 9.887 1.00 41.93

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MOTA 4413 CD ARG 570 9.182 1.00 49.89 51.459 2.966 **ATOM** 4414 NE ARG 570 52.329 2.991 8.009 1.00 55.25 **ATOM** 4416 CZARG 570 53.121 4.008 7.693 1.00 57.90 ATOM 4417 NH1 ARG 570 53.145 5.093 8.455 1.00 56.93 MOTA 4420 NH2 ARG 53.921 570 3.920 6.637 1.00 57.58 **ATOM** 4423 С ARG 570 53.219 -0.835 9.278 1.00 39.84 MOTA 4424 0 ARG 570 52.309 -1.644 9.060 1.00 42.48 **ATOM** 4425 N GLU 571 54.208 -0.597 8.425 1.00 38.22 **ATOM** 4427 CA GLU 571 54.292 -1.251 7.135 1.00 38.84 **ATOM** 4428 CB GLU 571 55.284 -0.492 6.266 1.00 40.72 MOTA 4429 CG GLU 571 54.818 0.941 5.999 1.00 49.17 **ATOM** 4430 CD GLU 571 55.845 1.798 5.284 1.00 58:95 MOTA 4431 OE1 GLU 571 1.434 __57.047 5.278 1.00 67.07 **ATOM** OE2 GLU 4432 571 55.455 2.854 4.736 1.00 61.02 ATOM C 4433 571 GLU 54.617 -2.744 7.240 1.00 37.79 MOTA 0 4434 GLU 571 54.075 -3.558 6.488 1.00 37.63 ATOM 4435 N TYR 572 55.462 -3.104 8.204 1.00 36.89 **ATOM** 4437 CA TYR 572 55.841 -4.498 8.437 1.00 36.81 MOTA 4438 CB TYR 572 56.822 -4.584 9.612 1.00 33.24 **ATOM** 4439 CG TYR 572 -5.987 57.191 10.080 1.00 33.42 **ATOM** 4440 CD1 TYR 572 -6.714 58.209 9.450 1.00 31.93 . ATOM 4441 CE1 TYR 572 58.623 -7.960 9.936 1.00 30.14 **ATOM** 4442 CD2 TYR 572 56.586 -6.552 11.208 1.00 34.42 ATOM 4443 CE2 TYR 572 56.991 -7.799 11.704 1.00 32.29 MOTA CZ -8.495 4444 TYR 572 58.012 11.965 1.00 32.52 **ATOM** 4445 OH TYR 572 58.427 -9..717 11.571 1.00 31.70 MOTA 4447 C TYR 572 54.588 -5.310 8.754 1.00 37.64 MOTA 4448 o TYR 572 54.387 -6.410 8.226 1.00 35.70 **ATOM** N 4449 LEU 53.742 573 -4.740 9.608 1.00 38.63 MOTA 4451 CA LEU 573 52.498 -5.376 10.011 1.00 38.21 MOTA 4452 CB LEU 573 51.802 -4.532 11.067 1.00 35.40 **ATOM** 4453 LEU CG 573 52.494 -4.421 12.419 1.00 34.55 MOTA 4454 CD1 LEU 573 51.755 -3.402 13.258 1.00 32.02 ATOM 4455 CD2 LEU 573 52.537 -5.788 13.108 1.00 34.58 MOTA 4456 С LEU 573 51.570 -5.549 8.818 1.00 38.11 MOTA 4457 0 LEU 573 51.144 -6.656 8.507 1.00 37.68 MOTA 4458 GLN N 574 51.286 -4.448 8.138 1.00 40.92 MOTA 4460 CA GLN 574 50.402 -4.476 6.982 1.00 45.16 MOTA 4461 CB GLN 574 50.213 -3.071 6.447 1.00 44.16 **ATOM** 4462 CG GLN 574 49.380 -2.239 7.369 1.00 45.26 MOTA 4463 CD GLN 574 49.222 -0.849 6.863 1.00 47.09 MOTA 4464 OE1 GLN 574 49.789 -0.483 5.838 1.00 50.83 MOTA 4465 NE2 GLN 574 48.450 -0.051 7.573 1.00 48.95 **ATOM** С 4468 GLN 574 50.807 -5.419 5.861 1.00 45.21 MOTA 4469 0 GLN 574 49.951 -6.031 5.215 1.00 49.63 MOTA 4470 N ALA 575 52.105 -5.562 5.646 1.00 43.35 MOTA 4472 CA ALA 575 52.579 -6.446 4.604 1.00 42.62 MOTA 4473 CB ALA 575 54.023 -6.130 4.284 1.00 43.49 **MOTA** 4474 C ALA 575 52.439 -7.906 5.022 1.00 42.85 **ATOM** 4475 0 ALA 575 52.771 -8.804 4.254 1.00 44.43 MOTA 4476 N ARG 576 51.937 -8.142 6.229 1.00 42.24 ATOM 4478 CA ARG 576 51.787 -9.494 6.747 1.00 41.58

MOTA	4479	СВ	ARG	5 7 6	52.813	- 9 . 725	7.849	1.00 40.10
MOTA	4480	CG	ARG	576	54.225	-9.694	7.314	1.00 40.58
ATOM	4481	CD	ARG	576	55.280	-9.604	8.392	1.00 42.40
ATOM	4482	NE	ARG	576	56.632	-9.607	7.826	1.00 41.95
ATOM	4484	CZ	ARG	576	57.110	-8.684	5.992	1.00 38.22
ATOM	4485	NH1	ARG	576	56.359	-7.658	6.612	1.00 38.61
ATOM	4488	NH2	ARG	576	58.347	~8.787	6.541	1.00 34.50
ATOM	4491	С	ARG	576	50.389	-9.762	7.255	1.00 43.28
MOTA	4492	0	ARG	576	50.187	-10.607	8.137	1.00 43.76
ATOM	4493	N	ARG	577	49.418	-9.057	6.684	1.00 44.65
ATOM	4495	CA	ARG	577	48.023	-9.222	7.C77	1.00 46.69
MOTA	4496	CB	ARG	577	47.197	-8.032	6.587	1.00 45.24
ATOM	4497	CG	ARG	577	47.372	-6.793	-7.440	1.00 42.93
MOTA	4498	CD	ARG	577	46.572	-5.635	6.898	1.00 44.63
ATOM	4499	NE	ARG	577	46.428	-4.577	7.895	1.00 47.76
ATOM	4501	CZ	ARG	577	45.750	-3.450	7.704	1.00 48.55
ATOM	4502	NHl	ARG	577	45.149	-3.225	6.548	1.00 50.64
MOTA	4505	NH2	ARG	577	45.643	-2.560	8.684	1.00 50.77
ATOM	4508	С	ARG	577	47.408	-10.540	6.603	1.00 47.12
ATOM	4509	O	ARG	577	47.396	-10.840	5.406	1.00 48.37
MOTA	4510	N	Gl-N	594	53.246	-13.595	7.891	1.00 64.66
ATOM	4512	CA	GLN	594	52.054	-13.835	8.728	1.00 65.10
ATOM	4513	CB	GLN .	594	51.130	-14.931	8.184	1.00 65.77
ATOM	4514	C	GLN	594	52.447	-14.127	10.174	1.00 64.01
MOTA	4515	0	GLN	594	52.962	-15.201	10.507	1.90 64.42
ATOM	4516	N	LEU	595	52.189	-13.154	11.031	1.00 61.45
MOTA	4518	CA	LEU	595	52.524	-13.245	12.437	1.00 59.21
ATOM	4519	CB	LEU	595	52.669	-11.826	12.979	1.00 57.54
ATOM	4520	CG	LEU	59 5	53.648	-11.043	12.099	1.00 56.37
ATOM	4521	CD1		595	53.442	-9.551	12.202	1.00 57.06
ATOM	4522	CD2	LEU	595	55.064	-11.430	12.465	1.00 55.57
ATOM	4523	C	LEU	595	51.509	-14.046	13.257	1.00 58.34
MOTA	4524	0	LEU	595	50.316	-14.039	12.953	1.00 58.21
ATOM	4525	N	SER	596	52.007	-14.740	14.280	1.00 58.00
ATOM	4527	CA	SER	596	51.182	-15.543	15.180	1.00 56.04
ATOM	4528	CB	SER	596	51.960	-16.770	15.667	1.00 57.98
ATOM	4529	OG	SER	596		-16.403	16.580	1.00 58.94
ATOM	4531	C	SER	596		-14.681	16.383	1.00 54 65
ATOM	4532	0	SER	596	51.479	-13.645	16.584	1.00 52.05
ATOM	4533	N	SER	597		-15.133	17.208	1.00 56.10
ATOM	4535	CA	SER	597		-14.389	18.398	1.00 57.51
ATOM	4536	CB	SER	597	48.530	-15.196	19.236	1.00 58.60
ATOM	4537	OG	SER	597		-15.914	18.421	1.00 61.95
ATOM	4539	С	SER	597	50.778	-14.094	19.220	1.00 57.75
ATOM	4540	0	SER	597		-12.998	19.755	1.00 57.86
ATOM	4541	N	LYS	598	51.692	-15.062	19.271	1.00 57.88
ATOM	4543	CA	LYS	598		-14.905	20.026	1.00 57.51
ATOM	4544	CB	LYS	598	53.690	-16.231	20.124	1.00 57.72
ATOM	4545	CG	LYS	598	54.470	-16.395	21.432	1.00 60.14
ATOM	4546	CD	LYS	598	55.227	-17.724	21.479	1.00 62.23
MOTA	4547	CE	LYS	598	55.894	-17.989	22.834	1.00 60.79
ATOM	4548	NZ	LYS	598	54.921	-18.149	23.949	1.00 61.46

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598 **ATOM** 4552 C LYS 53.809 -13.829 19.389 1.00 55.94 **MOTA** 4553 LYS 20.089 0 598 54.322 -12.955 1.00 55.84 4554 MOTA N ASP 599 53.935 -13.866 18.061 1.00 53.32 ATOM 4556 CA ASP 54.737 -12.882 17.334 599 1.00 50.30 1.00 49.72 **ATOM** 4557 CB ASP 599 54.688 -13.119 15.823 4558 **ATOM** ASP 55.426 -14.383 15.394 1.00 53.97 CG 599 **ATOM** 4559 OD1 ASP 16.214 599 56.176 -14 948 1.00 58.12 **ATOM** OD2 ASP 4560 599 55.261 -14.822 14.233 1.00 55.58 **ATOM** 4561 C ASP 599 54.247 -11.474 17.636 1.00 49.53 MOTA 0 1.00 51.16 4562 ASP 599 55.054 -10.589 17.911 **ATOM** 4563 N LEU 600 52.930 ~11.281 17.634 1.00 47.50 ATOM CA LEU -9.972 4565 600 52.354 17.909 1.00 45.41 MOTA 4566 CB LEU -9.948 600 50.850 17.627 1.00 43.77 ATOM 4567 CG LEU 600 50.429 -10.121 16.169 1.00 41.05 ATOM 4568 CD1 LEU 600 48.941 -9 904 16.048 1.00 41.04 MOTA 4569 CD2 LEU 600 51.160 -9 140 15.294 1.00 39.59 MOTA 4570 C LEU 600 52.638 -9.485 19.318 1.00 46.77 MOTA 4571 O LEU 600 -8.308 52.964 19.497 1.00 48.74 MOTA 4572 N VAL 601 52.524 -10.372 20 314 1.00 47.64 ATOM 4574 CA VAL 52.804 -10.002 601 21.716 1.00 47.38 MOTA 4575 CB VAL 601 52.321 -11.070 22.756 1.00 46.58 **ATOM** 4576 CG1 VAL 601 52.081 -10.403 24.114 1.00 45.07 ATOM 4577 VAL CG2 601 51.059 -11.759 22.306 1.00 48.86 **ATOM** 4578 C VAL 601 54.321 -9.811 21.890 1.00 46.04 MOTA -8.935 4579 Õ VAL 601 54.793 22.622 1.00 46.13 MOTA 4580 N SER 602 55.090 -10.624 21.183 1.00 44.21 **ATOM** 4582 21.233 CA SER 602 56.534 -10.546 1.00 42.78 ATOM 4583 CB SER 602 57.119 ~11.594 20.297 1.00 43.98 MOTA 4584 OG SER 602 58.523 -11.615 20.355 1.00 51.02 ATOM 4586 C SER 602 56.954 ~9.135 20.813 1.00 41.74 ATOM 4587 0 SER 602 57.709 -8.467 21.524 1.00 44.09 **ATOM** 4588 N CYS 603 56.425 -8.667 19.685 1.00 39.57 **MOTA** 4590 CA CYS 603 56.699 -7.317 19.177 1.00 36.11 **ATOM** 4591 CB **CYS** 603 -7.058 17.924 55.852 1.00 34.72 **ATOM** 4592 SG **CYS** 603 55.760 -5.364 17.323 0.50 29.10 PRT1 MOTA 4593 С **CYS** 603 56.378 -6.272 20.252 1.00 34.50 MOTA 4594 0 CYS 603 57.174 -5.371 20.506 1.00 33.61 MOTA 4595 N ALA 604 -6.429 20.913 55.236 1.00 34.64 **ATOM** 4597 CA ALA 604 54.811 -5.506 21.964 1.00 37.18 ATOM 4598 CB ALA 604 53.386 -5.850 22.414 1.00 38.20 ATOM 4599 С ALA 604 55.786 -5.516 23.160 1.00 38.91 MOTA 4600 O ALA 604 56.026 -4.481 23.790 1.00 38.29 MOTA 4601 N TYR 605 -6.693 56.323 23.477 1.00 39.54 MOTA 4603 CA TYR 605 57.283 -6.854 24.565 1.00 39.29 ATOM 4604 CB TYR 605 -8.340 57.573 24.791 1.00 40.07 ATOM 4605 CG TYR 605 -8.622 58.663 25.807 1.00 39.09 4606 **ATOM** CD1 TYR 605 58.525 -8.236 27.137 1.00 38.50 MOTA 4607 CE1 TYR 605 59.526 ~8.505 28.074 1.00 40.76 **ATOM** 4608 CD2 TYR 605 59.831 -9.283 25.435 1.00 39.73 MOTA 4609 CE2 TYR 605 60.B34 -9.553 26.361 1.00 37.45 MOTA 4610 CZTYR 605 60.678 -9.166 27.677 1.00 40.34 ATOM 4611 OH TYR 605 61.666 -9.466 28.601 1.00 43.16

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MOTA	4613	С	TYR	605	58.582	-6.113	24.224	1.00 39.45
MOTA	4614	0	TYR	605	59.067	-5.291	25.022	1.00 38.75
ATOM	4615	N	GLN	606	59.129	-6.410	23.040	1.00 36.41
MOTA	4617	CA	GLN	606	60.361	-5.787	22.550	1.00 35.20
MOTA	4618	CB	GLN	606	60.695	-6.303	21.150	1.00 34.86
MOTA	4619	CG	GLN	606	61.286	~7.695	21.118	1.00 32.21
MOTA	4620	CD	GLN	606	61.502	-8.205	19.709	1.00 32.63
ATOM	4621	OE1		606	62.495	-7.888	19.075	1.00 32.16
ATOM	4622		GLN	606	60.568	-9.004	19.216	1.00 34.62
MOTA	4625	C	GLN	606	60.286	-4.252	22.525	1.00 36.03
MOTA	4626	0	GLN	606	61.209	-3.572	22.989	1.00 38.81
ATOM	4627	N	VAL	607	59:188	-3.716	21.998	1.00 33.45
_ATOM	4629	CA	VAL	607	58.979	-2.280	21.923	1.00 29.34
MOTA	4630	CB	VAL	607	57.651	-1.948	21 189	1.00 28.80
ATOM	4631	CG1		607	57.260	-0.495	21.401	1.00 26.68
ATOM	4632		VAL	607	57.790	-2.244	19.€99	1.00 24.66
ATOM	4633	С	VAL	607	58.965	-1.698	23.339	1.00 31.35
ATOM	4634	C	VAL	607	59.557	-0.643	23.579	1.00 33.86
ATOM	4635	N	ALA	608	58.317	-2.402	24.270	1.00 30.17
MOTA	4637	CA	ALA	608	58.235	-1.971	25.667	1.00 28.98
ATOM	4638	CB	ALA	608	57.255	-2.836	26.440	1.00 28.30
ATOM	4639	C	ALA	608	59.598	-1.979	26.352	1.00 28.94
ATOM	4640	0	ALA	608	59.889	-1.091	27.155	1.00 27.83
ATOM	4641	Ŋ	ARG	609	60.435	-2.959	26.032	1.00 28.79
ATOM	4643	CA	ARG	609	51.765	-3.023	26.628	1.00 30.90
ATOM	4644	CB	ARG	609	62.499	-4.291	26.206	1.00 35.84
MOTA	4645	CG	ARG	609	51.787	-5.571	26.527	1.00 41.94
ATOM	4646	CD	ARG	609	62.782	-6.707	26.575	1.00 44.70
ATOM	4647	NE	ARG	609	63.392	-6.821	27.900	1.00 47.13
ATOM ATOM	4649	CZ	ARG	609	64.444	7.589	28.183	1.00 48.71
ATOM	4650		ARG	609	65.025	-3.314	27.233	1.00 48.33
ATOM	4653 4656	NH2 C	ARG	609	64.897	-7.655	29.428	1.00 49.11
ATOM	4657		ARG	609	62.602	-1.815	25.207	1.00 32.38
ATOM	4658	o N	ARG GLY	609	63.215	-1.148	27.058	1.00 32.63
ATOM	4660	CA		610 610	52.636	-1.554	24.894	1.00 29.98
ATOM	4661	CA	GLY GLY	610 610	63.384	-0.430	24.358	1.00 25.65
ATOM	4662	0	GLY	610	62.969	0.837	25.061	1.00 25.44
ATOM	4663	N	MET	611	63.791 61.672	1.640	25.463	1.00 27.09
ATOM	4665	CA	MET	611	61.167	1.009	25.242	1.00 30.41
ATOM	4666	СВ	MET	611	59.653	2.176	25.943	1.00 31.34
ATOM	4667	CG	MET	611	59.195	2.233	25.832	1.00 28.39
ATOM	4668	SD	MET	611	59.904	2.595 4.182	24.449	1.00 25.17
ATOM	4669	CE	MET	611	59.458	5.158	24.005	1.00 26.65
ATOM	4670	C	MET	611	61.600	2.176	25.453 27.412	1.00 19.78 1.00 34.05
ATOM	4671	ō	MET	611	62.008	3.211		
ATOM	4672	N	GLU	612	61.500	1.026	27.929 28.078	1.00 33.79
ATOM	4674	CA	GLU	612	61.893	0.913	29.484	1.00 37.16
ATOM	4675	CB	GLU	612	61.732	-0.533		1.00 38.85
ATOM	4676	CG	GLU	612	62.249	-0.533	29.988	1.00 38.96
ATOM	4677	CD	GLU	612	62.316	-2.271	31.400 31.783	1.00 35.19
ATOM	4678	OE1		612	62.605	-3.123		1.00 35.26
		~	-LU	VI2	02.005	~J.123	30.912	1.00 29.29

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ATOM 4679 OE2 GLU 612 62.102 -2.588 32.982 1.00 37.85 MOTA 4680 GLU 1.00 40.01 С 612 63.353 1.364 29.628 2.060 MOTA 4681 0 GLU 612 63.720 30.584 1.00 38.27 **ATOM** 4682 N TYR 613 64.176 0.972 28.662 1.00 40.33 **ATOM** 65.575 4684 CA TYR 613 1.362 28.664 1.00 39.71 **ATOM** 4685 CB TYR 66.333 0.722 613 27.494 1.00 39.03 ATOM 4686 67.800 CG TYR 613 1.100 27.467 1.00 41.41 **ATOM** 4687 68.702 CD1 TYR 613 0.527 28.364 1.00 42.79 MOTA 4688 CE1 TYR 613 70.048 0.905 28.386 1.00 40.21 MOTA 4689 CD2 TYR 68.283 2.068 613 26.581 1.00 39.75 **MOTA** 4690 CE2 TYR 613 69.621 2.454 26.596 1.00 39.01 **ATOM** 4691 CZ TYR 613 70.499 1.868 -27.503 1.00 39.56 MOTA 4692 OH TYR 613 71.823 2.249 27.538 1.00 35.63 ATOM 4694 C TYR 613 65.642 2.881 28.562 1.00 38.71 MOTA 4695 0 TYR 613 66.106 3.541 29.486 1.00 38.52 **ATOM** 4696 N LEU 614 65.126 3.423 27.460 1.00 37.22 **ATOM** 4698 CA LEU 614 65.128 4.864 27.212 1.00 35.66 **ATOM** 4699 CB LEU 64.223 614 5.202 26.025 1.00 35.27 MOTA 4700 CG LEU 614 64.687 4.699 24.659 1.00 33.09 **ATOM** 4701 CD1 LEU 63.718 1.00 33.31 614 5.188 23.612 MOTA 4702 CD2 LEU 614 66.099 5.184 24.363 1.00 31.20 **ATOM** 4703 LEU 64.672 1.00 35.64 C 614 5.653 28.430 MOTA 4704 0 LEU 614 65.298 6.639 28.816 1.00 34.54 ATOM 4705 N ALA 63.577 615. 5.203 29.032 1.00 36.61 ATOM 4707 CA ALA 615 63.028 5.835 30.222 1.00 37.74 ATOM 4708 CB ALA 615 61.682 -5.187 30.608 1.00 37.74 ATOM 4709 64.021 С ALA 615 5.776 31.389 1.00 37.30 **ATOM** 4710 0 64.111 ALA 615 6.731 32.175 1.00 37.29 MOTA 4711 N SER 616 64.752 4.665 31.511 1.00 37.18 ATOM 4713 CA 65.741 SER 616 4.534 32.577 1.00 36.92 ATOM 4714 CB SER 616 66.274 3.091 32.702 1.00 34.82 ATOM 4715 67.106 OG SER 616 2.680 31.628 1.00 28.79 ATOM 4717 C 66.870 SER 616 5.516 32.287 1.00 38.57 **ATOM** 4718 0 SER 67.633 616 5.902 33.179 1.00 38.30 MOTA 4719 LYS 66.958 N 617 5.925 31.024 1.00 37.62 MOTA 4721 CA LYS 617 67.965 6.876 30.606 1.00 36.13 MOTA 4722 CB LYS 617 68.511 6.494 29.238 1.00 35.90 MOTA 4723 CG LYS 617 69.274 5.206 29.236 1.00 34.58 MOTA 4724 CD LYS 617 70.502 5.348 30.077 1.00 35.44 MOTA 4725 CE LYS 617 71.201 4.022 30.232 1.00 38.54 MOTA 4726 NZ LYS 617 72.566 4.211 30.790 1.00 41.54 ATOM 4730 С LYS 617 67.378 8.275 30.564 1.00 36.55 MOTA 4731 0 LYS 617 67.943 9.155 29.934 1.00 40.26 MOTA 4732 N LYS 618 66.221 8.468 31.187 1.00 36.42 ATOM 4734 CA LYS 618 65.570 9.779 31.231 1.00 36.06 MOTA 4735 CB LYS 618 66.543 10.B33 31.746 1.00 42.22 MOTA 4736 CG LYS 618 67.234 10.499 33.062 1.00 52.36 ATOM 4737 CD LYS 618 66.301 10.668 1.00 61.51 34.236 MOTA 4738 CE LYS 618 66.933 10.121 35.495 1.00 67.28 **ATOM** 4739 NZ LYS 618 65.965 10.161 36.618 1.00 73.99 ATOM 4743 C LYS 618 65.026 10.261 29.887 1.00 34.94 ATOM 4744 LYS 618 64.562 0 11.393 29.781 1.00 34.69

ATOM	4745	N	CYS	619	65.051	9.407	28.872	1.00	34.46
ATOM	4747	CA	CYS	619	64.588	9.793	27.543		33.12
ATOM	4748	CB	CYS	619	65.311	8.966	26.475		34.33
ATOM	4749	SG	CYS	619	64.920	9.397	24.778		35.64
ATOM	4750	С	CYS	619	63.075	9.699	27.355		32.13
MOTA	4751	0	CYS	619	62.465	8.645	27.584		30.72
MOTA	4752	N	ILE	620	62.477	10.818	26.960	1.00	32.70
MOTA	4754	CA	ILE	620	61.046	10.909	26.708		32.75
MOTA	4755	CB	ILE	620	60.440	12.129	27.421	1.00	33.55
ATOM	4756	CG2	ILE	620	59.002	12.339	26.986	1.00	38.39
ATOM	4757	CG1		620	60.486	11.913	28.933	1.00	30.71
ATOM	4758	CD1		620	59.994	13.084	29.710	1.00	30.11
ATOM	4759	C	ILE	- 620-	···60.969 ·	11.086	25.206	1.00	33.31
ATOM	4760	O	ILE	620	61.516	12.040	24 674	1.00	33.40
ATOM	4761	N	HIS	621	60.356	10.114	24.533	1.00	33.56
ATOM	4763	CA	HIS	621	60.230	10.092	23.087	1.00	32.30
ATOM	4764	CB	HIS	621	59.866	8.668	22.642	1.00	29.55
MOTA	4765	CG	HIS	621	60.049	8.402	21.173	1.60	27.32
ATOM	4766		HIS	621	60.694	7.404	20.533	1.00	24.26
ATOM ATOM	4767		HIS	621	59.462	9.173	20.187	1.00	25.20
ATOM	4769		HIS	621	59.734	8.652	19.006	1.00	25.81
ATOM	4770 4772	C C	HIS	621	60.481	7.579	19.184	1.00	26.65
ATOM	4773	U	HIS	621	59.246	11.103	22.499		35.40
ATOM	4774	N	HIS ARG	621 622	59.459	11.574	21.388		39.18
ATOM	4776	CA	ARG	622	58.128	11.363	23.178	1.00	
ATOM	4777	CB	ARG	622	57.117 57.694	12.323	22.686		36.40
ATOM	4778	CG	ARG	622	58.171	13.732	22.617		35.62
ATOM	4779	CD	ARG	622	58.837	14.253 15.591	23.937	1.00	
ATOM	4780	NE	ARG	622	59.315	16.101	23.759 25.032		32.17
ATOM	4782	CZ	ARG	622	60.487	15.786	25.575	0.50	32.82
ATOM	4783	NH1	ARG	622	61.326	14.965	24.952	0.50	
ATOM	4786	NH2	ARG	622	60.803	16.268	26.769		32.70
MOTA	4789	C	ARG	622	56.405	12.008	21.355	1.00	
ATOM	4790	0	ARG	622	55.527	12.763	20.936	1.00	
ATOM	4791	N	ASP	623	56.806	10.938	20.668		35.84
ATOM	4793	CA	ASP	623	56.128	10.538	19.436	1.00	
MOTA	4794	CB	ASP	623	56.574	11.352	18.221	1.00	
ATOM	4795	CG	ASP	623	55.736	11.036	16.974	1.00	
ATOM	4796	OD1	ASP	623	56.277	11.082	15.851	1.00	
MOTA	4797	OD2	ASP	623	54.535	10.715	17.119	1.00	50.45
ATOM	4798	С	ASP	623	56.271	9.052	19.162	1.00	32.98
ATOM	4799	0	ASP	623	56.664	8.645	18.073	1.00	30.90
ATOM	4800	N	LEU	624	56.015	8.244	20.179	1.00	31.16
ATOM	4802	CA	LEU	624	56.099	6.801	20.029	1.00	31.71
ATOM	4803	CB.	LEU	624	56.070	6.144	21.407	1.00	
ATOM	4804	CG	LEU	624	56.049	4.618	21.514	1.00	28.13
ATOM	4805	CD1		624	57.225	3.975	20.799	1.00	27.00
ATOM	4806	CD2		624	56.072	4.283	22.987	1.00	29.10
MOTA	4807	C	LEU	624	54.917	6.320	19.185	1.00	
ATOM	4808	0	LEU	624	53.763	6.608	19.508	1.00	
MOTA	4809	N	ALA	625	55.214	5.640	18.081	1.00	29.82

ATOM	4811	CA	ALA	625	54.194	5.106	17.181	1.00 28.29
MOTA	4812	CB	ALA	625	53.682	6.182	16.245	1.00 26.72
ATOM	4813	C	ALA	625	54.895	4.031	16.395	1.00 28.40
ATOM	4814	0	ALA	625	56.118	4.028	16.343	1.00 32.12
ATOM	4815	N	ALA	626	54.131	3.135	15.770	1.00 28.55
MOTA	4817	CA	ALA	626	54.687	2.028	14.979	1.00 26.25
MOTA	4818	CB	ALA	626	53.577	1.169	14.365	1.00 23.54
MOTA	4819	С	ALA	626	55.569	2.573	13.892	1.00 23.68
ATOM	4820	0	ALA	626	56.544	1.944	13.519	1.00 26.07
ATOM	4821	N	ARG	627	55.208	3.744	13.378	1.00 23.80
ATOM	4823	CA	ARG	627	55.980	4.413	12.338	1.00 26.57
ATOM	4824	CB	ARG	627	55.289	5.728	11.914	1.00 25.91
MOTA	4825	CG	ARG	627	54.991	6.692	13.055	1.00 27.60
MOTA	4826	CD	ARG	627	54.711	8.130	12.584	1.00 33.01
MOTA	4827	NE	ARG	627	54.260	8.978	13.691	1.00 34.18
ATOM	4829	CZ	ARG	627	52.997	9.067	14.091	1.00 35.88
ATOM	4830	NH1	ARG	627	52.056	8.380	13.460	1.00 38.89
ATOM	4833	NH2	ARG	627	52.689	9.748	15.183	1.00 36.43
ATOM	4836	С	ARG	627	57.439	4.686	12.785	1.00 29.03
ATOM	4837	0	ARG	627	58.362	4.606	11.972	1.00 29.24
ATOM	4838	N	ASN	628	57.634	4.938	14.087	1.00 29.51
ATOM	4840	CA	ASN	628	58.954	5.234.	14.645	1.00 26.41
ATOM	4841	CB	ASN	628	58.864	5.359	15.676	1.00 25.32
MOTA	4842	CG	ASN	628	58.539	7.687	15.035	1.00 28.11
ATOM	4843	OD1	ASN	628	59.079	8.028	13.999	1.00 32.09
ATOM	4844	ND2	ASN	628	57.639	8.426	15.628	1.00 27.88
ATOM	4847	C	ASN	628	59.684	4.039	15.225	1.00 25.77
ATOM	4848	O	ASN	628	60.641	4.188	16.001	1.00 24.77
ATOM	4849	N	VAL	629	59.209	2.853	14.874	1.00 26.63
ATOM	4851	CA	VAL	629	59.828	1.610	15.315	1.00 25.34
ATOM	4852	CB	VAL	629	58.812	0.693	16.007	1.00 21.26
ATOM	4853		VAL	629	59.492	-0.604	16.412	1.00 22.96
ATOM	4854		VAL	629 .	58.205	1.398	17.207	1.00 16.65
MOTA	4855	C	VAL	629	60.266	0.1962	14.007	1.00 26.79
ATOM	4856	0	VAL	629	59.454	0.839	13.087	1.00 28.60
ATOM	4857	N	LEU	630	61.542	0.603	13.904	1.00 25.91
ATOM	4859	CA	LEU	630	62.062	-0.021	12.685	1.00 26.95
ATOM	4860	CB	LEU	630	63.297	0.733	12.210	1.00 22.79
ATOM	4861	CG	LEU	630	63.044	2.242	12.111	1.00 20.04
ATOM	4862	CD1	LEU	630	64.345	2.944	11.972	1.00 11.86
ATOM	4863	CD2		630	62.111	2.603	10.965	1.00 19.22
MOTA	4864	С	LEU	630	62.367	-1.492	12.961	1.00 28.01
ATOM	4865	0	LEU	630	62.629	-1.852	14.101	1.00 28.26
ATOM	4866	N	VAL	631	62.246	-2.346	11.946	1.00 30.82
ATOM	4868	CA	VAL	631	62.468	-3.790	12.098	1.00 31.75
ATOM	4869	CB	VAL	631	61.194	-4.607	11.659	1.00 30.04
ATOM	4870	CG1		631	61.346	-6.085	12.026	1.00 29.25
ATOM	4871	CG2		631	59.937	-4.030	12.290	1.00 24.59
ATOM	4872	C	VAL	631	63.697	-4.286	11.305	1.00 35.24
ATOM	4873	0	VAL	631	63.849	-3.999	10.097	1.00 34.02
MOTA	4874	N	THR	632	64.551	-5.052	11.979	1.00 36.24
ATOM	4876	CA	THR	632	65.770	-5.574	11.365	1.00 38.23

ATOM	4877	CB	THR	632	66.843	-5.836	12.416	1.00 38.21
ATOM	4878	OG1	THR	632	66.423	-6.908	13.272	1.00 38.31
ATOM	4880	CG2	THR	632	67.069	-4.582	13.238	1.00 40.22
MOTA	4881	С	THR	632	65.526	-6.854	10.593	1.00 39.17
ATOM	4882	0	THR	632	64.471	-7.457	10.744	1.00 41.26
ATOM	4883	N	GLU	633	66.496	-7.259	9.766	1.00 41.23
MOTA	4885	CA	GLU	633	66.397	-8.483	8.960	1.00 42.62
MOTA	4886	CB	GLU	633	67.677	-8.712	8.154	1.00 44.25
ATOM	4887	CG	GLU	633	67.610	-9.884	7.154	1.00 51.05
ATOM	4888	CD	GLU	633	66.825	-9.594	5.858	1.00 56.28
ATOM	4889	OE1	GLU	633	66.390	-8.444	5.626	1.00 62.64
ATOM	4890	OE2	GLU	633	66.651	-10.536	5.058	1.00 58.41
ATOM	4891	C	GLU	633	66.097	-9.722	9.797	1.00 41.83
ATOM	4892	0	GLU	633	65.578	-10.704	9.288	1.00 42.77
MOTA	4893	N	ASP	634	66.415	-9.665	11.082	1.00 43.14
ATOM	4895	CA	ASP	634	66.167	-10.784	11.978	1.00 44.01
ATOM	4896	CB	ASP	634	67.361	-11.007	12.914	1.00 49.37
ATOM	4897	CG	ASP	634	68.636	-11.396	12.166	1.09 54.70
ATOM	4898	OD1		634	68.683	-12.515	11.595	1.00 55.43
ATOM	4899	OD2		634	69.602	-10.596	12.167	1.00 56.17
ATOM	4900	C	ASP	634	64.925	-10.507	12.801	1.00 43.95
MOTA	4901	0	ASP	634	64.754	-11.085	13.864	1.00 45.92
ATOM	4902	N	ASN	635	64.075	-9.604	12.316	1.00 44.71
ATOM	4904	CA	ASN	635	62.822	-9.220	12.980	1.00 43.07
ATOM	4905	CB	ASN	635	61.854	-10.404	13.018	1.00 45.50
ATOM	4906	CG	ASN	635	51.606	-10.994	11.653	1.00 45.43
ATOM	4907	OD1		635		-10.369	10.788	1.00 49.56
ATOM	4908	ND2		635		-12.190	11.435	1.00 48.18
ATOM ATOM	4911	C	ASN	635	62.927	-8.609	14.380	1.00 41.64
ATOM	4912	0	ASN	635	62.050	-8.814	15.221	1.00 41.69
ATOM	4913 4915	N CA	VAL	636	63.984	-7.843	14.627	1.00 41.17
ATOM	4916	CB	VAL VAL	636 636	64.177	-7.178	15.922	1.00 39.01
ATOM	4917	CG1		636	65.692	-7.002 -6.200	16.259	1.00 40.66
ATOM	4918	CG2		636	65.882 66.355	-5.209	17.560	1.00 35.04
ATOM	4919	C	VAL	636	63.544	-8.360 -5.789	16.367 15.925	1.00 41.69
ATOM	4920	ō	VAL	636	63.817	-4.989	15.925	1.00 36.77
ATOM	4921	N	MET	637	62.696	~5.518	16.908	1.00 38.35 1.00 35.71
ATOM	4923	CA	MET	637	62.049	-4.216	17.031	1.00 35.71 1.00 33.65
ATOM	4924	СВ	MET	637	60.783	-4.319	17.884	1.00 33.65
MOTA	4925	CG	MET	637	59.737	-5.314	17.371	1.00 38.24
MOTA	4926	SD	MET	637	59.128	-4.993	15.695	1.00 42.24
ATOM	4927	CE	MET	637	59.249	-6.621	14.976	1.00 39.27
ATOM	4928	C	MET	637	63.001	-3.209	17.668	1.00 32.62
MOTA	4929	0	MET	637	63.524	-3.436	18.765	1.00 30.56
ATOM	4930	N	LYS	638	63.173	-2.070	17.008	1.00 30.38
ATOM	4932	CA	LYS	638	64.073	-1.027	17.492	1.00 32.03
ATOM	4933	СВ	LYS	638	65.351	-1.027	16.654	1.00 27.71
ATOM	4934	CG	LYS	638	66.245	-2.211	16.896	1.00 27.71
ATOM	4935	CD	LYS	638	67.429	-2.170	15.976	1.00 24.50
ATOM	4936	CE	LYS	638	68.443	-3.187	16.390	1.00 22.85
ATOM	4937	NZ	LYS	638	69.121	-2.803	17.651	1.00 24.79
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ATOM	4941	С	LYS	638	63.443	0.364	17.446	1.00 28.00
ATOM	4942	0	LYS	638	62.977	0.799	16.391	1.00 25.60
ATOM	4943	N	ILE	639	63.410	1.032	18.601	1.00 25.32
ATOM	4945	CA	ILE	639	62.857	2.379	18.721	1.00 25.91
ATOM	4946	CB	ILE	639	62.800	2.875	20.201	1.00 25.56
ATOM	4947	CG2	ILE	639	62.074	4.208	20.279	1.00 22.82
ATOM	4948	CG1	ILE	639	62.142	1.835	21.118	1.00 28.00
ATOM	4949	CD1	ILE	639	60.634	1.748	21.003	1.00 33.25
ATOM	4950	С	ILE	639	63.739	3.363	17.955	1.00 26.87
ATOM	4951	0	ILE	639	64.968	3.381	18.125	1.00 24.13
ATOM	4952	N	ALA	640	63.108	4.170	17.108	1.00 26.74
ATOM	4954	CA	ALA	640	63.825	5.176	16.339	1.00 30.62
ATOM	4955	СВ	ALA	640	63.624	4.939	14.851	100 30.31
АТОМ	4956	С	ALA	640	63.338	6.572	16.739	1.00 32.53
A.TOM	4957	0	ALA	640	62.289	6.706	17.371	1.00 33.83
ATOM	4958	N	ASP	641	64.082	7.605	16.351	1.00 33.05
ATOM	4960	CA	ASP	641	63.749	9.010	16.656	1.00 37.66
MOTA	4961	СВ	ASP	641	62.539	9.489	15.840	1.00 42.62
ATOM	4962	CG	ASP	641	62.928	10.026	14.471	1.00 50.92
ATOM	4963		ASP	641	64.092	9.833	14.021	1.00 59.21
ATOM	4964		ASP	641	62.063	10.652	13.823	1.00 54.05
ATOM	4965	С	ASP	641	63.545	9.367	18.125	1.00 37.85
ATOM	4966	o	ASP	641	62.805	10.294	18.448	1.00 39.10
ATOM	4967	N	PHE	642	64.204	8.635	19.016	1.00 37.47
ATOM	4969	CA	PHE	642	64.099	8.874	20.456	1.00 36.47
ATOM	4970	CB	PHE	642	64.403	7.581	21.226	1.00 32.22
ATOM	4971	CG	PHE	642	65.786	7.013	20.964	1.00 30.65
ATOM	4972	CD1	PHE	642	66 . 906	7.537	21.607	1.00 32.45
ATOM	4973	CD2	PHE	642	65.969	5.981	20.054	1.00 28.53
ATOM	4974	CE1	PHE	642	68.180	7.050	21.342	1.00 30.88
ATOM	4975	CE2	PHE	642	67.234	5.494	19.789	1.00 27.74
ATOM	4976	CZ	PHE	642	68.344	6.027	20.431	1.00 29.64
ATOM	4977	C	PHE	642	65.050	10.001	20.907	1.00 39.69
MOTA	4978	0	PHE	642	64.967	10.469	22.047	1.00 38.22
MOTA	4979	N	GLY	643	65.966	10.400	20.015	1.00 41.08
MOTA	4981	CA	GLY	643	66.925	11.447	20.324	1.00 40.65
MOTA	4982	С	GLY	643	66.694	12.747	19.571	1.00 43.53
MOTA	4983	0	GLY	643	67.500	13.666	19.688	1.00 41.10
MOTA	4984	N	LEU	644	65.617	12.825	18.786	1.00 48.35
MOTA	4986	CA	LEU	644	65.306	14.034	18.019	1.00 51.11
MOTA	4987	CB	LEU	644	63. 96 2	13.907	17.314	1.00 50.28
ATOM	4988	CG	LEU	644	63.900	13.059	16.057	1.00 54.03
MOTA	4989	CD1	LEU	644	62.541	13.278	15.413	1.00 57.34
ATOM	4990	CD2	LEU	644	65.006	13.467	15.105	1.00 56.95
ATOM	4991	С	LEU	644	65.248	15.257	18.894	1.00 52.68
ATOM	4992	0	LEU	644	64.850	15.175	20.053	1.00 54.95
ATOM	4993	N	ALA	645	65629	16.399	18.332	1.00 54.61
ATOM	4995	CA	ALA	645	65.610	17.656	19.073	1.00 54.60
MOTA	4996	CB	ALA	645	66.495	18.684	18.382	1.00 53.32
ATOM	4997	С	ALA	645	64.178	18.185	19.215	1.00 54.09
ATOM	4998	0	ALA	645	63.716	18.488	20.322	1.00 53.14
ATOM	4999	N	ASP	652	52.340	21.795	14.895	1.00 91.33

ATOM	5001	CA	ASP	652	51.194	21.914	14.004	1.00 90.97
MOTA	5002	СВ	ASP	652	51.650	22.138	12.555	1.00 92.06
MOTA	5003	CG	ASP	652	50.488	22.434	11.606	1.00 94.00
MOTA	5004	OD1	ASP	652	49.479	23.032	12.042	1.00 95.25
ATOM	5005	OD2	ASP	652	50.586	22.075	10.414	1.00 94.81
ATOM	5006	С	ASP	652	50.352	20.652	14.103	1.00 90.61
MOTA	5007	0	ASP	652	50.645	19.641	13.463	1.00 91.26
ATOM	5008	N	TYR	653	49.289	20.737	14.895	1.00 89.65
ATOM	5010	CA	TYR	653	48.381	19.619	15.110	1.00 88.25
ATOM	5011	CB	TYR	653	47.306	20.003	16.133	1.00 88.16
ATOM	5012	CG	TYR	653	47.800	20.140	17.559	1.00 88.74
MOTA	5013	CD1	TYR	653	47.047	20.818	18.513	1.00 90.00
ATOM	5014	CE1	TYR	653	47.477	20.915	19.839	1::00 90:70
ATOM	5015	CD2	TYR	653	49.006	19.559	17.964	1.00 89.14
ATOM	5016	CE2	TYR	653	49.443	19.649	19.280	1.00 89.49
ATOM	5017	CZ	TYR	653	48.675	20.325	20.214	1.00 89.80
ATOM	5018	OH	TYR	653	49.109	20.394	21.518	1.00 89.81
ATOM	5020	С	TYR	653	47.701	19.165	13.830	1.00 87.32
MOTA	5021	0	TYR	653	47.180	18.057	13 759	1 00 87.70
ATOM	5022	N	TYR	654	47.734	20.013	12.814	1.00 86.51
ATOM	5024	C'A	TYR	654	47.087	19.707	11.553	1.00 87.08
ATOM	5025	CB	TYR	654	46.387	20.959	11.028	1 00 88.45
ATOM	5026	CG	TYR	654	45.375	21.497	12.014	1.00 90.25
ATOM	5027	CD1	TYR	654	45.781	22.017	13.246	1.00 90.15
ATOM	5028		TYR	654	44.857	22.431	14.197	1.00 90 94
ATOM	5029	CD2	TYR	654	44.012	21.419	11.753	1.00 91.22
MOTA	5030	CE2	TYR	654	43.078	21.833	12.698	1.00 93.22
ATOM	5031	CZ	TYR	654	43.506	22.335	13.918	1.00 92.39
MOTA	5032	OH	TYR	654	42.588	22.717	14.872	1.00 94.38
ATOM ATOM	5034	Ĉ	TYR	654	48.C12	19.115	10.503	1.00 87.34
ATOM	5035	0	TYR	654	47.567	18.767	9.410	1.00 88.29
ATOM	5036 5038	N	LYS	655	49.290	18.971	10.836	1.00 86.67
ATOM	5039	CA CB	LYS	655 655	50.233	18.406	9.987	1.00 87.62
ATOM	5040	CG	LYS LYS	655 655	51.666	18.814	10.229	1.00 90.01
ATOM	5040	CD	LYS	655 655	52.688	18.252	9.251	1.00 95.23
ATOM	5042	CE	LYS	655	54.106	18.646	9.607	1.00 99.04
ATOM	5042	NZ	LYS	655	55.108	17.832	8.789	1.00102.26
ATOM	5047	C	LYS	655	56.528	18.184	9.099	1.00104.44
ATOM	5048	0	LYS	655	50.102 50.233	16.890	9.896	1.00 87.61
ATOM	5049	N	LYS	656	49.787	16.259 16.319	10.945	1.00 87.58
ATOM	5051	CA	LYS	656	49.639	14.875	8.737 8.603	1.00 87.88
ATOM	5052	СВ	LYS	656	48.795	14.537	7.376	1.00 89.03
ATOM	5053	CG	LYS	656	47.313	14.802	7.535	1.00 90.44
ATOM	5054	CD	LYS	656	46.590	14.599		1.00 93.30
ATOM	5055	CE	LYS	656	45.089	14.555	6.213 6.406	1.00 96.87
ATOM	5056	NZ	LYS	656	44.362	14.535	5.106	1.00 99.35
ATOM	5060	C	LYS	656	51.004	14.318	8.487	1.00102.42 1.00 88.57
ATOM	5061	0	LYS	656	51.004	14.749	7.855	
ATOM	5062	N	GLY	660	49.270	10.021	5.735	1.00 88.38 1.00 61.58
ATOM	5064	CA	GLY	660	48.416	11.168	6.005	1.00 51.58
ATOM	5065	C	GLY	660	47.664	11.100	7.324	1.00 58.75
		-			47.004	11,000	1.344	1.00 57.22

ATOM	5066	0	GLY	660	46.555	11.624	7.437	1.00 58.01
ATOM	5067	N	ARG	661	48.231	10.374	8.293	1.00 55.37
ATOM	5069	CA	ARG	661	47.631	10.247	9.622	1.00 51.19
ATOM	5070	CB	ARG	661	48.095	8.965	10.337	1.00 51.89
ATOM	5071	CG	ARG	661	47.756	7.663	9.612	1.00 51.56
ATOM	5072	CD	ARG	661	48.057	6.443	10.484	1.00 50.77
MOTA	5073	NE	ARG	661	47.834	5.181	9.772	1.00 50.04
ATOM	5075	CZ	ARG	661	48.015	3.974	10.307	1.00 48.12
ATOM	5076	NH1	ARG	661	48.421	3.855	11.569	1.00 43.28
ATOM	5079	NH2	ARG	661	47.788	2.882	9.578	1.00 43.69
ATOM	5082	C	ARG	661	48.041	11.463	10.446	1.00 46.22
, ATOM	5083	0	ARG	661	48.998	12.162	10.097	1.00 44.78
MOTA	5084	N	LEU	662	47.328	11.703	11.542	1.00 41.80
MOTA	5086	CA	LEU	662	47.621	12.837	12.419	1.00 36.78
MOTA	5087	CB	LEU	662	46.342	13.596	12.758	1.00 33.05
MOTA	5088	CG	LEU	662	45.642	14.279	11.585	1.00 28.24
ATOM	5089	CD1	LEU	662	44.198	147.611	11.935	1.00 24.66
ATOM	5090	CD2	LEU	662	46.429	15.511	11.217	1.00 28.35
ATOM	5091	C	LEU	662	48.278	12.328	13.695	1.00 36.10
ATOM	5092	O	LEU	662	47.695	11.521	14.431	1.00 34.46
MOTA	5093	N	PRO	663	49.526	12.751	13.945	1.00 35.83
ATOM	5094	CD	PRO	663	50.360	13.537	13.022	1.00 37.72
MOTA	5095	CA	PRO	663	50.310	12.365	15.119	1.00 35.68
ATOM	5096	CB	PRO	663	51.611	13.130	14.914	1.00 35.23
MOTA	5097	CG	PRO	663	51.756	13.134	13.437	1.00 36.10
ATOM	5098	C	PRO	663	49.660	12 703	16.453	1.00 35.87
ATOM	5099	0	PRO	663	49.958	12.069	17.469	1.00 39.86
ATOM	5100	N	VAL	664	48.787	13.705	16.466	1.00 33.54
ATOM	5102	CA	VAL	664	48.109	14.076	17.699	1.00 31.24
ATOM	5103	CB	VAL	664	47.196	15.321	17.520	1.00 30.45
ATOM	5104	CG1	VAL	664	48.025	16.480	17.051	1.00 32.54
ATOM	5105	CG2	VAL	664	46.093	15.062	16.523	1.00 34.77
ATOM	5106	C	VAL	664	47.301	12.895	18.233	1.00 31.33
MOTA	5107	0	VAL	664	47.095	12.782	19.438	1.00 32.66
MOTA	5108	N	LYS	665	46.940	11.968	17.345	1.00 30.44
MOTA	5110	CA	LYS	665	46.153	10.795	17.719	1.00 28.43
ATOM	5111	CB	LYS	665	45.596	10.133	16.466	1.00 24.82
ATOM	5112	CG	LYS	665	44.700	11.086	15.687	1.00 27.50
MOTA	5113	CD	LYS	665	44.096	10.466	14.442	1.00 26.62
MOTA	5114	CE	LYS	665	42.967	11.326	13.909	1.00 21.64
MOTA	5115	NZ	LYS	665	42.479	10.850	12.584	1.00 25.29
MOTA	5119	C	LYS	665	46.889	9.794	18.615	1.00 29.56
ATOM	5120	0	LYS	665	46.295	8.836	19.095	1.00 29.57
ATOM	5121	N	TRP	666	48.183	10.020	18.826	1.00 30.12
ATOM	5123	CA	TRP	666	48.987	9.174	19.704	1.00 31.39
MOTA	5124	CB	TRP	666	50.329	8.845	19.059	1.00 30.40
ATOM	5125	CG	TRP	666	50.263	7.700	18.106	1.00 30.79
MOTA	5126	CD2	TRP	666	49.701	7.719	16.785	1.00 30.22
MOTA	5127	CE2		666	49.891	6.430	16.245	1.00 28.24
ATOM	5128	CE3	TRP	666	49.067	8.702	16.012	1.00 30.60
ATOM	5129	CD1		666	50.743	6.435	18.307	1.00 28.07
ATOM	5130	NE1		666	50.522	5.670	17.187	1.00 29.15
						2.370	,	

ATOM	5132	CZ2	TRP	666	49.462	6.107	14.954	1.00 29.38
ATOM	5133	CZ3	TRP	666	48.640	8.374	14.726	1.00 31.27
ATOM	5134	CH2	TRP	666	48.845	7.086	14.213	1.00 31.33
MOTA	5135	С	TRP	666	49.242	9.902	21.026	1.00 33.92
ATOM	5136	0	TRP	666	49.591	9.287	22.040	1.00 35.23
MOTA	5137	N	MET	667	49.028	11.214	21.007	1.00 35.72
MOTA	5139	CA	MET	667	49.260	12.065	22.159	1.00 36.43
MOTA	5140	CB	MET	667	49.163	13.529	21.751	1.00 37.70
MOTA	5141	CG	MET	667	50.510	14.194	21.574	1.00 40.10
MOTA	5142	SD	MET	667	50.358	15.906	21.096	1.00 46.91
MOTA	5143	CE	MET	667	50.914	15.810	19.386	1.00 40.40
ATOM	5144	C	MET	667	48.389	11.839	23.378	1.00 38.36
MOTA	5145	0	MET	667	47.186	11.646	23.273	1.00 39.53
ATOM	5146	N	ALA	668	49.027	11.885	24.542	1.00 39.93
ATOM	5148	CA	ALA	668	48.345	11.733	25.815	1.00 38.48
ATOM	5149	CB	ALA	668	49.351	11.537	26.929	1.00 37.61
ATOM	5150	C	ALA	668	47.603	13.038	26.014	1.00 39.48
ATOM	5151	С	ALA	668	48.059	14.090	25.566	1.00 39.40
MOTA	5152	N	PRO	669	46.474	13.001	26.731	1.00 42.22
MOTA	5153	CD	PRO	669	45.842	11.827	27.355	1.00 42.77
MOTA	5154	CA	PRO	669	45.677	14.204	26.980	1.00 43.91
MOTA	5155	CB	PRO	669	44.609	13.698	27.948	1.00 44.49
ATOM	5156	CG	PRO	669	44.421	12.279	27.499	1.00 43.59
ATOM	5157	С	PRO	669	46.476	15.372	27.570	1.00 44.89
ATOM	5158	O	PRO	669	46.394	16.497	27.075	1.00 45.48
ATOM	5159	N	GLU	670	47.266	15.105	28.607	1.00 43.39
ATOM	5161	CA	GLU	670	48.050	16.158	29.244	1.00 42.97
ATOM	5162	CB	GLU	670	48.739	15.645	30.504	1.00 43.31
ATOM	5163	CG	GLU	670	49.864	14.646	30.252	1.00 44.78
ATOM	5164	CD	GLU	670	49.408	13.204	30.290	1.00 43.48
ATOM	5165	OE1		670	50.225	12.331	30.639	1.00 41.85
ATOM	5166	OE2		670	48.235	12.931	29.986	1.00 47.18
ATOM	5167	С	GLU	670	49.090	16.798	28.333	1.00 43.18
ATOM	5168	0	GLU	670	49.362	17.983	28.444	1.00 41.68
ATOM	5169	N	ALA	671	49.677	16.00B	27.440	1.00 44.65
ATOM	5171	CA	ALA	671	50.686	16.512	26.513	1.00 44.44
ATOM	5172	CB	ALA	671	51.412	15.347	25.841	1.00 40.17
ATOM	5173	C	ALA	671	50.046	17.410	25.465	1.00 46.49
ATOM	5174	0	ALA	671	50.558	18.484	25.148	1.00 45.70
ATOM	5175	N	LEU	672	48.903	16.970	24.952	1.00 50.30
ATOM	5177	CA	LEU	672	48.163	17.702	23.925	1.00 52.07
ATOM	5178	CB	LEU	672	47.080	16.782	23.335	1.00 54.41
ATOM	5179	CG	LEU	672	46.388	17.103	22.005	1.00 57.12
MOTA	5180	CD1		672	47.404	17.316	20.912	1.00 57.65
ATOM	5181	CD2		672	45.459	15.951	21.640	1.00 56.14
ATOM	5182	C .	LEU	672	47.535	18.964	24.512	1.00 52.42
ATOM	5183	0	LEU	672	47.683	20.058	23.969	1.00 52.71
MOTA	5184	N	PHE	673	46.863	18.803	25.645	1.00 52.74
ATOM	5186	CA	PHE	673	46.203	19.911	26.314	1.00 54.32
ATOM	5187	CB	PHE	673	44.995	19.394	27.104	1.00 52.92
MOTA	5188	CG	PHE	673	43.987	18.646	26.259	1.00 52.38
MOTA	5189	CD1	PHE	673	43.399	17.477	26.728	1.00 53.49

5190 MOTA CD2 PHE 24.999 1.00 51.61 673 43.624 19.109 MOTA CE1 PHE 5191 25.957 673 42.468 16.779 1.00 50.49 MOTA 5192 CE2 PHE 673 42.698 18.420 24.229 1.00 50.91 **ATOM** 5193 CZPHE 673 42.118 17.250 24.710 1.00 50.09 20.732 **ATOM** 5194 C PHE 673 27.220 47.138 1.00 56.29 ATOM. 5195 0 PHE 673 27.026 47.289 21.938 1.00 58.05 **ATOM** 5196 N ASP 28.165 674 47.808 20.076 1.00 56.38 **ATOM** 5198 CA ASP 674 48.703 20.772 29.104 1.00 56.12 **ATOM** 5199 CB ASP 674 48.644 20.101 30.485 1.00 53.81 MOTA 5200 CG ASP 674 47.299 20.234 31.152 1.00 52.48 ATOM 5201 OD1 ASP 674 46.715 19.188 31.504 1.00 50.25 MOTA 5202 OD2 ASP 674 46.844 21.384 31.337 1.00 51.16 MOTA 5203 С ASP 674 50.182 20.886 28.706 1.00 57.07 ATOM 5204 0 ASP 674 51.010 21.273 29.541 1.00 56.00 **ATOM** 5205 N ARG 675 50.525 20.526 27.468 1.00 57.28 ATOM 5207 CA ARG 675 51.915 20.576 26.995 1.00 55.64 ATOM 5208 CB ARG 675 52..341 22.020 26.692 1.00 58.95 MOTA 5209 CG ARG 675 51.542 22.678 25.559 1.00 66.91 ATOM 5210 CD ARG 675 52.082 24.066 25.202 1.00 72.90 MOTA 5211 NE ARG 675 24.019 24.482 53.360 1.00 75.10 ATOM 5213 CZARG 1.00 73.61 675 54.096 25.089 24.181 ATOM 5214 NH1 ARG 675 53.687 26.301 24.536 1.00 71.27 **ATOM** 5217 NH2 ARG 675 55.250 24.943 23.540 1.00 72.12 ATOM 5220 С ARG 19.932 675 52.853 28.017 1.00 53.25 MOTA 5221 0 ARG 675 53.988 20.366 28.211 1.00 52.13 MOTA 5222 N ILE 676 52.359 18.883 28.664 1.90 51.44 ATOM 5224 CA ILE 676 53.108 18.153 29.683 1.00 49.81 MOTA 5225 CB ILE 676 52.241 17.944 30.958 1.00 46.07 **ATOM** 5226 CG2 ILE 676 52.804 16.844 31.856 1.00 40.98 **ATOM** 5227 CG1 ILE 676 52.129 19.257 31.721 1.00 43.31 ATOM 5228 CD1 ILE 676 51.324 19.147 32.963 1.00 45.02 **ATOM** 5229 C ILE 676 53.572 16.800 29.144 1.00 51.20 **ATOM** 5230 0 ILE 676 52.770 15.892 28.951 1.00 52.37 **ATOM** 5231 N TYR 677 54.865 16.675 28.890 1.00 52.81 **ATOM** 5233 CA TYR 677 55.412 15.429 28.383 1.00 53.96 MOTA 5234 CB TYR 677 27,167 56.296 15.700 1.00 57.26 **ATOM** 5235 CG TYR 677 55.524 16.175 25.951 1.00 64.10 MOTA 5236 CD1 TYR 677 55.229 17.532 25.762 1.00 65.60 MOTA 5237 CE1 TYR 677 54.514 17.965 24.634 1.00 67.15 **ATOM** 5238 CD2 TYR 677 55.085 15.263 24.985 1.00 66.29 MOTA 5239 CE2 TYR 677 54.376 15.680 23.862 1.00 67.34 MOTA 5240 CZTYR 677 54.095 17.028 23.692 1.00 69.24 **ATOM** 5241 OH TYR 677 53.399 17.414 22.573 1.00 73.55 **ATOM** 5243 С TYR 677 56.192 14.713 29.482 1.00 52.30 MOTA 5244 TYR 0 677 57.053 15.309 30.124 1.00 53.73 ATOM 5245 N THR 678 55.830 13.461 29.748 1.00 48.95 **ATOM** 5247 CA THR 56.505 12.659 678 30.760 1.00 45.99 MOTA 5248 CB THR 678 55.729 12.634 32.107 1.00 46.04 **ATOM** 5249 OG1 THR 678 54.663 11.676 32.046 1.00 49.79 **ATOM** 5251 CG2 THR 678 55.160 14.010 32.429 1.00 45.58 **ATOM** 5252 THR C 56.656 678 11.221 30.261 1.00 43.81 MOTA 5253 THR 0 678 56.231 10.888 29.158 1.00 45.12

ATOM	5254	N	HIS	679	57.250	10.359	31.076	1.00 41.50
ATOM	5256	CA	HIS	679	57.414	8.971	30.687	1.00 38.39
MOTA	5257	CB	HIS	679	58.390	8.253	31.603	1.00 38.62
MOTA	5258	CG	HIS	679	59.798	8.770	31.524	1.00 41.51
ATOM	5259	CD2	HIS	679	60.456	9.690	32.273	1.00 40.12
MOTA	5260	NDl	HIS	679	60.715	8.296	30.613	1.00 41.18
MOTA	5262	CE1	HIS	679	61.880	8.892	30.806	1.00 39.44
MOTA	5263	NE2	HIS	679	61.747	9.742	31.807	1.00.41.37
MOTA	5265	C	HIS	679	56.068	8.279	30.720	1.00 39.57
MOTA	5266	0	HIS	679	55.909	7.215	30.137	1.00 41.93
MOTA	5267	N	GLN	680	55.108	8.863	31.429	1.00 39.84
MOTA	5269	CA	GLN	680	53.773	8.290	31.483	1.00 38.92
ATOM	5270	CB	GLN	680	53.021	8.705-	32.751	1.00 38.21
ATOM	5271	CG	GLN	680	53.518	8.005	34.022	1.00 42.17
ATOM	5272	CD	GLN	680	53.651	6.477	33.879	1.00 43.35
ATOM	5273	OE1	GLN	680	52.686	5.737	34.056	1.00 44.05
ATOM	5274	NE2	GLN	680	54.860	6.010	33.564	1.00 37.17
ATOM	5277	С	GLN	680	53.012	8.674	30.221	1.00 39.33
ATOM	5278	0	GLN	680	52.220	7.883	29.709	1.00 40.26
ATOM	5279	N	SER	681	53.299	9.854	29.673	1.00 38.00
ATOM	5281	CA	SER	681	52 636	10.251	28.441	1.00 37.44
ATOM	528 2	CB	SER	681	52 963	11.698	28.078	1.00 37.67
ATOM	5283	OG	SER	681	54.349	11.937	28.302	1.00 38.03
MOTA	5285	С	SER	681	53.095	9.278	27.356	1.00 38.28
MOTA	5286	0	SER	681	52.302	8.866	26.510	1.00 39.41
ATOM	5287	N	ASP	682	54.362	8.866	27.431	1.00 36.81
ATOM	5289	CA	ASP	682	54.920	7.888	26.495	1.30 36.41
ATOM	5290	CB	ASP	682	56.404	7.655	26.765	1.00 37.18
MOTA	5291	CG.	ASP	682	57.309	8.584	25.968	1.00 40.08
ATOM	5292		ASP	682	58.528	8.317	25.959	1.00 41.94
ATOM	5293		ASP	682	56.824	9.565	25.352	1.00 39.55
ATOM ATOM	5294	C	ASP	682	54.180	6.561	26.645	1.00 36.93
ATOM	5295	0	ASP	682	54.005	5.818	25.675	1.00 38.23
ATOM	5296 5298	N CA	VAL	683	53.742	6.268	27.866	1.00 36.33
ATOM	5299	CB	VAL VAL	683	53.000	5.040	28.143	1.00 36.29
ATOM	5300		VAL	683 683	52.834	4.820	29.683	1.00 35.29
ATOM	5301		VAL	683	51.900	3.653	29.989	1.00 34.98
ATOM	5302	C	VAL	683	54.198	4.546	30.312	1.00 30.55
ATOM	5302	0	VAL	683	51.648	5.067	27.392	1.00 35.21
ATOM	5304	N	TRP	684	51.223	4.050	26.845	1.00 32.81
ATOM	5304	CA	TRP	684	51.027 49.759	6.245	27.309	1.00 34.49
ATOM	5307	СВ	TRP	684		6.412	26.602	1.00 36.39
ATOM	5308	CG	TRP	684	49.200 48.006	7.825	26.811	1.00 39.30
ATOM	5309		TRP	684	46.651	8.174	25.947	1.00 41.47
ATOM	5310		TRP	684	45.896	8.381	26.384	1.00 42.41
ATOM	5311		TRP	684	46.004	8.744	25.247	1.00 41.76
ATOM	5311		TRP	684		8.298	27.627	1.00 42.06
ATOM	5312	NE1		684	48.010 46.749	8.410	24.597	1.00 40.55
ATOM	5315		TRP	684		8.756	24.175	1.00 42.32
ATOM	5316		TRP	684	44.522	9.022	25.315	1.00 41.35
ATOM					44.638	8.576	27.692	1.00 41.99
AION	5317	CHZ	TRP	684	43.917	8.933	26.541	1.00 41.07

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MOTA	5318	C	TRP	684	49.964	6.125	25.115	1.00 36.12
MOTA	5319	0	TRP	684	49.152	5.410	24.511	1.00 38.69
MOTA	5320	N	SER	685	51.029	6.690	24.534	1.00 33.48
ATOM	5322	CA	SER	685	51.395	6.491	23.130	1.00 26.49
MOTA	5323	CB	SER	685	52.636	7.300	22.802	1.00 23.40
ATOM	5324	OG	SER	685	52.403	8.688	22.992	1.00 30.31
ATOM	5326	С	SER	685	51.665	5.015	22.859	1.00 26.25
MOTA	5327	0	SER	685	51.377	4.510	21.782	1.00 28.78
ATOM	5328	N	PHE	686	52.214	4.319	23.846	1.00 28.14
MOTA	5330	CA	PHE	686	52.470	2.884	23.727	1.00 28.53
ATOM	5331	CB	PHE	686	53.245	2.399	24.947	1.00 27.34
ATOM	5332	CG	PHE	686	53.567	0.937	24.917	1.00 29.91
ATOM	5333		PHE	686	54.424	0.419	23.942	.100 29.23
ATOM	5334		PHE	686	53.016	0.075	25.861	1.00 28.28
MOTA	5335		PHE	686	54.725	-0.936	23.908	1.00 27.65
ATOM	5336	CE2	PHE	686	53.307	-1.274	25.840	1.00 27.18
ATOM	5337	CZ	PHE	686	54.166	-1.787	24.861	1.00 30.06
ATOM	5338	C	PHE	686	51.129	2.117	23.618	1.00 31.42
ATOM	5339	0	PHE	686	51.041	1.096	22.930	1.00 29.05
ATOM	5340	N	GLY	687	50.093	2.623	24.298	1.00 31.18
ATOM	5342	CA	GLY	687	48.783	2.000	24258	1.00 32.16
ATOM	5343	C	GLY	687	48.276	2.026	22.825	1.00 35.09
ATOM	5344	0	GLY	687	47.805	1.011	22.289	1.00 36.38
ATOM	5345	h	VAL	688	48.378	3.188	22.186	1.00 33.72
ATOM	5347	CA	VAL	688	47.949	3.307	20.808	1.00 30.28
ATOM	5348	CB	VAL	688	47.996	4.761	20.322	1.60 28.62
ATOM	5349	CG1		688	47.433	4.862	18.905	1.00 26.79
ATOM	5350	CG2		688	47.202	5.645	21.275	1.00 26.40
ATOM	5351	C	VAL	588	48.823	2.406	19.930	1.00 30.01
ATOM	5352	0	VAL	688	48.324	1.782	18.989	1.00 30.37
ATOM ATOM	5353	N CA	LEU	689	50.108	2.282	20.273	1.00 29.76
ATOM	5355 5356	CB	LEU	689 689	51.022	1.418	19.510	1.00 29.37
ATOM	5357	CG	LEU		52.476 53.564	1.577 0.944	19.982 19.097	1.00 25.78
ATOM	5358	CD1		689	54.855	1.741	19.057	1.00 23.00 1.00 24.44
ATOM	5359	CD2		689	53.823	-0.471	19.479	
ATOM	5360	C	LEU	689	50.583	-0.471	19.479	1.00 21.63 1.00 29.98
MOTA	5361	0	LEU	689	50.708	-0.806	18.678	1.00 28.75
ATOM	5362	N	LEU	690	50.048	-0.409	20.803	1.00 32.38
ATOM	5364	CA	LEU	690	49.562	-1.764	21.060	1.00 32.66
ATOM	5365	СВ	LEU	690	49.114	-1.929	22.517	1.00 32.33
ATOM	5366		LEU	690	50.107	-2.192	23.658	1.00 32.00
ATOM	5367	CD1		690	49.330	-2.201	24.962	1.00 35.74
ATOM	5368	CD2		690	50.834	-3.513	23.475	1.00 30.76
ATOM	5369		LEU	690	48.369	-2.018	20.156	1.00 33.29
ATOM	5370		LEU	690	48.248	-3.079	19.550	1.00 35.08
ATOM	5371	N	TRP	691	47.490	-1.026	20.065	1.00 34.28
ATOM	5373	CA	TRP	691	46.304	-1.114	19.221	1.00 33.79
ATOM	5374	СВ	TRP	691	45.483	0.172	19.364	1.00 32.68
ATOM	5375	CG	TRP	691	44.147	0.144	18.669	1.00 31.23
ATOM	5376	CD2		691	43.888	0.490	17.312	1.00 28.11
ATOM	5377	CE2		691	42.506	0.310	17.089	1.00 29.96
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MOTA	5378	CE3	TRP	691	44.686	0.949	16.257	1.00 28.70
ATOM	5379	CD1	TRP	691	42.936	-0.225	19.208	1.00 29.37
MOTA	5380	NE1	TRP	691	41.951	-0.130	18.265	1.00 30.89
MOTA	5382	CZ2	TRP	691	41.909	0.555	15.845	1.00 29.50
ATOM	5383	CZ3	TRP	691	44.093	1.194	15.021	1.00 27.43
ATOM	5384	CH2	TRP	691	42.719	1.002	14.830	1.00 29.27
ATOM	5385	С	TRP	691	46.744	-1.319	17.763	1.00 34.12
ATOM	5386	0	TRP	691	46.139	-2.088	17.029	1.00 33.88
ATOM	5387	N	GLU	692	47.817	-0.636	17.366	1.00 36.37
MOTA	5389	CA	GLU	692	48.355	-0.723	16.010	1.00 35.35
ATOM	5390	СВ	GLU	692	49.532	0.233	15.826	1.00 31.75
ATOM	5391	CG	GLU	692	49.138	1.694	15.746	1.00 32.63
ATOM ·	5392	-CD	GLU	692	50.318	2.585	15.403	1.00 35.28
ATOM	5393	OE1	GLU	692	51.150	2.847	16.301	1.00 37.81
MOTA	5394	OE2	GLU	692	50.430	3.017	14.237	1.00 34.85
ATOM	5395	C	GLU	692	48.810	-2.118	15.658	1.00 35.71
ATOM	5396	0	GLU	692	48.589	-2.570	14.544	1.00 37.26
ATOM	5397	N	ILE	693	49.439	-2.798	16.610	1.00 35.05
ATOM	5399	CA	ILE	693	49.944	-4.153	16.396	1.00 35.00
ATOM	5400	CB	ILE	693	50.843	-4.608	17.575	1.00 35.88
MOTA	5401	CG2	ILE	693	51.275	-6.064	17.400	1.00 36.03
MOTA	5402	CG1	ILE	693	52.081	-3.711	17.669	1.00 34.66
MOTA	5403	CD1	ILE	693	52.814	-3.874	18.943	1.00 35.52
ATOM	5404	C	ILE	693	48.810	-5.153	16.232	1.00 34.29
MOTA	5405	Ō	ILE	693	48.790	-5.943	15.281	1.00 33.66
MOTA	5406	N	PHE	694	47.837	-5. 07 9	17.127	1.00 34.44
MOTA	5408	CA	PHE	694	46.722	-5.999	17.682	1.00 35.63
MOTA	5409	CB	PHE	694	46.156	~6.167	18.490	1.00 35.26
ATOM	5410	CG	PHE	694 .	47.158	-6.787	19.428	1.00 35.26
ATOM	5411	CD1	PHE	694	47.796	-6.017	20.389	1.00 33.07
MOTA	5412	CD2	PHE	694	47.574	-8.111	19.237	1.00 31.74
ATOM	5413	CE1		694	48.837	-5.539	21.137	1.00 31.01
ATOM	5414	CE2	PHE	694	48.614	-8.643	19.982	1.00 31.64
ATOM	5415	CZ	PHE	694	49.254	-7.855	20.934	1.00 31.84
ATOM	5416	C	PHE	694	45.688	-5.771	15.986	1.00 36.62
ATOM	5417	0	PHE	694	44.844	-6.632	15.729	1.00 38.73
ATOM	5418	N	THR	695	45.781	-4.626	15.313	1.00 35.76
ATOM	5420	CA	THR	695	44.898	-4.331	14.191	1.00 34.86
ATOM	5421	CB	THR	695	44.245	-2.929	14.298	1.00 32.81
ATOM	5422	OG1	THR	695	45.246	-1.909	14.211	1.00 31.61
ATOM	5424		THR	695	43.497	~2.795	15.603	1.00 29.90
ATOM	5425	C	THR	695	45.766	-4.426	12.934	1.00 35.95
ATOM	5426	0	THR	695	45.333	-4.064	11.841	1.00 38.88
ATOM	5427	N	LEU	696	46.993	-4.919	13.119	1.00 34.68
ATOM	5429	CA	LEU	696	47.979	-5.100	12.053	1.00 32.84
ATOM	5430	CB	LEU	696	47.622	-6.294	11.161	1.00 32.65
ATOM	5431	CG	LEU	696	47.493	-7.657	11.838	1.00 30.89
ATOM	5432	CD1		696	47.315	-8.734	10.785	1.00 31.30
ATOM	5433	CD2		696	48.718	-7.939	12.659	1.00 30.76
ATOM	5434	С	LEU	696	48.280	-3.872	11.197	1.00 32.43
ATOM	5435	0	LEU	696	48.259	-3.931	9.965	1.00 31.48
ATOM	5436	N	GLY	697	48.597	-2.768	11.867	1.00 33.65

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697 **ATOM** 5438 CA GLY 48.940 -1.529 11.188 1.00 32.78 GLY 10.960 MOTA 5439 C 697 47.742 -0.641 1.00 33.06 MOTA 5440 O GLY 697 47.728 0.172 10.048 1.00 34.74 11.782 ATOM 5441 N GLY 698 46.719 -0.798 1.00 35.53 11.612 MOTA 5443 0.009 CA GLY 698 45.531 1.00 36.87 MOTA 5444 С GLY 698 45.771 1.496 11.753 1.00 34.92 ATOM 5445 0 GLY 698 46.779 1.926 12.299 1.00 34.08 **ATOM** 5446 N SER 699 44.814 2.271 11.265 1.00 36.45 **ATOM** 5448 CA SER 699 44.858 3.725 11.318 1.00 35.36 ATOM 5449 CB SER 699 44.363 4.290 9.995 1.00 34.58 10.087 **ATOM** 5450 OG SER 699 44.126 5.684 1.00 41.43 **ATOM** 5452 С SER 699 43.927 4.146 12.451 1.00 36.53 MOTA 5.45.3. O. SER 699 42.734 3.812 12.438 1.00 37.58._ MOTA 5454 N PRO 700 44.471 4.799 13.491 1.00 36.03 **ATOM** 5455 CD PRO 700 45.896 5.028 13.776 1.00 34.58 **ATOM** 5456 CA PRO 700 43.630 5.228 14.611 1.00 35.47 ATOM 5457 CB PRO 700 44.655 5.573 15.694 1.00 34.59 **ATOM** 5458 CG PRO 700 45.840 5.990 14.919 1.00 34.18 **ATOM** 5459 С PRO 700 42.742 6.411 14.247 1.00 34.66 **ATOM** 5460 0 PRO 700 43.194 7.363 13.616 1.00 34.39 MOTA 1.00 34.11 5461 N TYR 701 41.462 6 293 14.588 MOTA 5463 CA TYR 701 40.459 7.324 14.338 1.00 33.11 701 MOTA TYR 5464 CB 40.713 8..548 15.225 1.00 38.13 MOTA CG TYR 701 5465 40.552 8.272 16.706 1.00 43.52 **ATOM** CD1 TYR 701 5466 41.538 8.637 17.616 1.00 14.79 **ATOM** 546? CE1 TYR 701 41.387 8.391 18.978 1.00 49.99 ATOM 54*E*8 CD2 TYR 701 . 39.405 7.647 17.197 1.00 47.59 MOTA 5469 CE2 TYR 701 39.245 7.395 18.552 1.00 49 15 MOTA 5470 CZTYR 701 40.237 7.770 19.444 1.00 50.84 MOTA 5471 OH TYR 701 1.00 54.00 40.091 7.539 20.804 ATOM 5473 C TYR 701 7.736 12.877 40.389 1.00 30.95 MOTA 5474 0 TYR 701 12.534 40.597 8.900 1.00 30.64 ATOM 5475 N PRO 702 40.096 6.773 11.985 1.00 30.06 **ATOM** 5476 CD PRO 702 39.887 5.336 12.192 1.00 25.47 **ATOM** 5477 CA 702 PRO 40.014 7.112 10.561 1.00 29.36 ATOM 5478 CB PRO 702 39.836 5.744 9.899 1.00 25.86 MOTA 5479 CG PRO 702 4.946 10.929 39.185 1.00 24.42 MOTA 5480 C PRO 702 38.859 8.045 10.256 1.00 31.49 **ATOM** 5481 0 PRO 702 37.716 7.794 10.654 1.00 33.50 **ATOM** N 5482 GLY 703 39.194 9.151 9.592 1.00 30.85 **ATOM** 5484 CA GLY 703 38.210 10.149 9.212 1.00 27.67 ATOM 5485 С GLY 703 37.985 11.230 10.250 1.00 27.39 **MOTA** 5486 0 GLY 703 37.270 12.194 9.981 1.00 26.56 **ATOM** 5487 N VAL 704 11.100 38.627 11.412 1.00 27.05 **ATOM** 5489 VAL CA 704 12.053 38.466 12.505 1.00 28.50 ATOM 5490 VAL CB 704 38.576 11.364 13.876 1.00 28.95 ATOM 5491 CG1 VAL 704 38.509 12.397 14.990 1.00 29.36 MOTA 5492 CG2 VAL 704 37.475 10.338 14.045 1.00 29.64 MOTA 5493 С VAL 704 39.473 13.194 12.493 1.00 30.95 ATOM 5494 0 VAL 12.977 704 40.669 12.661 1.00 32.90 MOTA N PRO 5495 705 39.001 14.428 12.269 1.00 31.09 **ATOM** 5496 CD PRO 705 37.682 14.795 11.728 1.00 31.49

ATOM	5497	CA	PRO	705	39.926	15.561	12.255	1.00 29.66
ATOM	5498	CB	PRO	705	39.152	16.618	11.477	1.00 30.16
MOTA	5499	CG	PRO	705	37.720	16.289	11.778	1.00 33.76
MOTA	5500	C	PRO	705	40.334	16.028	13.654	1.00 29.25
MOTA	5501	0	PRO	705	39.693	15.695	14.659	1.00 24.77
MOTA	5502	N	VAL	706	41.396	16.828	13.690	1.00 32.40
MOTA	5504	CA	VAL	706	41.976	17.355	14.929	1.00 36.51
MOTA	5505	CB	VAL	706	43.023	18.450	14.629	1.00 36.79
ATOM	5506	CG1	VAL	706	43.680	18.903	15.914	1.00 37.79
MOTA	5507	CG2	VAL	706	44.058	17.942	13.653	1.00 37.26
MOTA	5508	C	VAL	706	40.977	17.915	15.943	1.00 38.21
ATOM	5509	0	VAL	706 .	41.052	17.600	17.130	100 37.65
ATOM	5510	N	GLU -	70-7	40:060	18.754	15.467	1.00 40.27
ATOM	5512	CA	GLU	707	39.045	19.360	16.324	1.00 40.57
MOTA	5 5 13	CE	GLU	707	38.186	20.324	15.499	1.00 40.56
MOTA	5514	C	GLU	707	38.164	18.288	16.958	1.00 41.60
ATOM	5515	0	GLU	707	37.871	18.323	18.158	1.00 41.79
ATOM	5516	N	GLU	708	37.784	17.311	16.143	1.00 42.54
ATOM	5518	CA	GLU	708	36.947	16.210	16.576	1.00 44.09
MOTA	5519	CB	GLU	708	36 509	15.398	15.367	1.00 47.61
MOTA	5520	CG	GLU	708	35.687	16.219	14.381	1.00 50.42
MOTA	5521	CD	GLU	708	34.511	16.891	15.042	1.00 55.51
ATOM	5522	OE1	GLU	708	33.856	16.249	15.899	1.00 58.91
ATOM	5523		GLU	708	34.244	18.067	14.714	1.00 60.06
ATOM	5524	C	GLU	708	37.661	15.338	17.598	1.00 44.63
ATOM	5525	O	GLU	708	37.058	14.893	18.585	1.00 45.12
ATOM	5526	N	LEU	709	38.9€0	15.141	17.390	1.00 43.72
MOTA	5528	C.A	LEU	709	39.768	14.346	18.312	1.00 39.85
MOTA	5529	CB	LEU	709	41.212	14.243	17.823	1.00 34.99
ATOM	5530	CG	LEU	709	42.037	13.359	18.756	1.00 31.80
ATOM	5531		LEU	709	41.519	11.918	18.598	1.00 29.20
ATOM	5532		LEU	709	43.495	13.533	18.454	1.00 31.19
ATOM	5533	C	LEU	709	39.751	15.001	19.683	1.00 39.26
ATOM	5534	0	LEU	709	39.646	14.317	20.714	1.00 37.71
ATOM	5535	N	PHE	710	39.872	16.327	19.691	1.00 38.62
MOTA	5537	CA	PHE	710	39.862	17.068	20.942	1.00 41.82
MOTA	5538	CB	PHE	710	40.016	18.567	20.688	1.00 42.02
ATOM	5539	CG	PHE	710	41.383	18,958	20.20€	1.00 43.81
ATOM	5540	CD1		710	42.441	18.043	20.242	1.90 47.07
ATOM	5541	CD2		710	41.621	20.234	19.718	1.00 42.91
ATOM ATOM	5542	CE1		710	43.716	18.401	19.793	1.00 49.22
ATOM	5543 5544	CE2		710	42.890	20.602	19.267	1.00 46.73
ATOM		CZ	PHE	710	43.942	19.681	19.307	1.30 48.40
	5545	C	PHE	710	38.568	16.787	21.698	1.00 43.80
ATOM ATOM	5546 5547	O N	PHE	710	38.593	16.502	22.904	1.00 44.54
ATOM		N.	LYS	711	37.452	16.790	20.968	1.00 44.15
ATOM	5549 5550	CA	LYS	711	36.148	16.539	21.569	1.00 42.60
ATOM		CB	LYS	711	35.029	16.855	20.577	1.00 44.35
ATOM	5551 5552	CG	LYS	711	33.661	16.781	21.200	1.00 48.05
ATOM	5553	CD CE	LYS	711	32.560	17.205	20.263	1.00 49.23
ATOM	5554		LYS	711	31.212	16.804	20.855	1.00 50.61
AION	2224	NZ	LYS	711	30.078	17.204	19.987	1.00 56.56

MOTA	5558	C	LYS	711	36.045	15.105	22.084	1.00 41.50
MOTA	5559	0	LYS	711	35.589	14.875	23.202	1.00 41.06
MOTA	5560	N	LEU	712	36.489	14.144	21.282	1.00 41.61
ATOM	5562	CA	LEU	712	36.463	12.737	21.687	1.00 43.22
MOTA	5563	CB	LEU	712	37.070	11.841	20.600	1.00 41.69
MOTA	5564	CG	LEU	712	36.246	11.404	19.397	1.00 38.07
ATOM	5565	CD1	LEU	712	37.071	10.460	18.527	1.00 34.55
ATOM	5566	CD2	LEU	712	34.990	10.714	19.891	1.00 37.28
MOTA	5567	С	LEU	712	37.253	12.536	22.982	1.00 43.94
MOTA	5568	0	LEU	712	36.804	11.832	23.900	1.00 41.71
ATOM	5569	N	LEU	713	38.444	13.129	23.029	1.00 45.26
ATOM	5571	CA	LEU	713	39.318	13.022	24.191	1.00 46.47
MOTA	5572	CB	LEU	713	40.647	13 728	23.925	1.90 46.32
ATOM	5573	CG	LEU	713	41.524	13.012	22.889	1.00 44.05
ATOM	5574	CD1	LEU	713	42.853	13.737	22.734	1.00 39.96
MOTA	5575	CD2	LEU	713	41 758	11.571	23.328	1.00 41.78
ATOM	5576	С	LEU	713	38.665	13.519	25.477	1.00 47.50
ATOM	5577	С	LEU	713	38.630	12.789	26.472	1.00 48.26
ATOM	5578	N	LYS	714	38.098	14.725	25.440	1.00 47.08
ATOM	5580	CA	LYS	714	37.41.9 .	15.302	26.600	1.00 45.59
ATOM	5581	СВ	LYS	714 .	36.974	16.727	26.293	1.00 47.53
MOTA	5582	CG	LYS	714	38.126	17.661	26.064	1.00 51.33
ATOM	5583	ന്മ	LYS	714	37.647	19.044	25.689	1.00 59.12
MOTA	5584	CE	LYS	714	38.836	19.917	25.273	1.00 64.39
ATOM	5585	NZ	LYS	714	39.843	20.072	26.370	1.00 66.31
MOTA	5589	C	LYS	714	36.217	14.476	27.056	1.00 44.19
MOTA	5590	0	LYS	714	35.895	14.447	28.244	1.00 43.04
MOTA	5591	Ñ	GLU	715	35.565	13.805	26.112	1.00 43.89
MOTA	5593	CA	GLU	715	34.401	12.976	26.424	1.00 44.12
MOTA	5594	CB	GLU	715	33.512	12.785	25.190	1.00 47.40
MOTA	5595	CG	GLU	715	32.860	14.053	24.623	1.00 52.31
MOTA	5596	CD	GLU	715	31.953	13.763	23.427	1.00 56.22
MOTA	5597	OE1	GLU	715	32.121	12.699	22.784	1.00 57.16
ATOM	5598	OE2	GLU	715	31.059	14.588	23.138	1.00 57.32
ATOM	5599	C	GLU	715	34.809	11.605	26.956	1.00 42.47
MOTA	5600	0	GLU	715	33.964	10.718	27.094	1.00 41.03
ATOM	5601	N	GLY	716	36.101	11.419	27.201	1.00 41.06
MOTA	5603	CA	GLY	716	36.593	10.150	27.718	1.00 41.58
MOTA	5604	С	GLY	716	36.548	8.985	26.739	1.00 41.60
ATOM	5605	0	GLY	716	36.640	7.816	27.141	1.00 38.34
ATOM	5606	N	HIS	717	36.469	9.303	25.450	1.00 42.80
ATOM	5608	CA	HIS	717	36.398	8.278	24.420	1.00 45.03
ATOM	5609	CB	HIS	717	36.082	8.894	23.052	1.00 46.28
ATOM	5610	CG	HIS	717	35.987	7.887	21.940	1.00 48.73
MOTA	5611	CD2		717	34.941	7.157	21.483	1.00 48.67
ATOM	5612	ND1		717	37.071	7.521	21.169	1.00 49.33
ATOM	5614	CE1		717	36.701	6.607	20.290	1.00 45.65
ATOM	5615	NE2		717	35.410	6.370	20.460	1.00 45.87
MOTA	5617	С	HIS	717	37.662	7.448	24.324	1.00 46.84
MOTA	5618	0	HIS	717	38.767	7.980	24.319	1.00 48.06
MOTA	5619	N	ARG	718	37.478	6.138	24.217	1.00 48.75
ATOM	5621	CA	ARG	718	38.573	5.181	24.091	1.00 49.16

ATOM	5622	СВ	ARG	718	38.694	4.345	25.370	1.00	46.96
MOTA	5623	CG	ARG	718	39.005	5.164	26.617	1.00	49.78
ATOM	5624	CD	ARG	718	40.344	5.891	26.474	1.00	52.81
ATOM	5625	NE	ARG	718	40.724	6.639	27.672	1.00	52.99
ATOM	5627	CZ	ARG	718	40.598	7.961	27.817	1.00	53.38
MOTA	5628		ARG	718	40.094	8.705	26.836	1.00	52.33
ATOM	5631	NH2	ARG	718	41.025	8.553	28.928	1.00	49.30
MOTA	5634	С	ARG	718	38.257	4.293	22.878	1.00	50.73
ATOM	5635	0	ARG	718	37.086	4.003	22.601	1.00	51.78
ATOM	5636	N	MET	719	39.286	3.899	22.136	1.00	50.83
ATOM	5638	CA	MET	719	39.086	3.072	20.948	1.00	50.56
ATOM	5639	CB	MET '	719	40.355	3.013	20.094	1.00	48.85
ATOM	5640	CG	MET	719	40.748	4.325	19.438	1.00	45.25
ATOM	5641	SD	MET	719	42.152	4.119	18.335	1.00	43.24
ATOM	5642	CE	MET	719	43.471	4.066	19.465	1.00	36.42
ATOM	5643	C	MET	719	38.649	1.671	21.312	1.00	51.07
ATOM	5644	0	MET	719	39.087	1.132	22.325	1.00	48.42
ATOM	5645	N	ASP	720	37.797	1.096	20.462	1.00	53.92
ATOM	5647	CA	ASP	720	37.254	-0.253	20.648	1.00	55.90
ATOM	5648	CB	ASP	720	36.221	-0.597	19.553	1.00	57.16
ATOM	5649	CG	ASP	720	34.998	0.320	19.552	1.00	59.05
ATOM	5650		ASP	720	34.951	1.316	20.312	1.00	63.29
ATOM	5651		ASP	720	34.0.74	0.042	18.758		54.85
ATOM	5652	C	ASP	720	38.326	-1.343	20.638		55.89
ATOM	5653	0	ASP	720	39.397	-1.190	20.927		55.28
ATOM	5654	Ŋ	LYS	721	38.009	-2.450	21.304		56.09
ATOM	5656	CA	LYS	721	38.892	-3.605	21.370	1.00	56.46
ATOM ATOM	5657	CB	LYS	721	38.344	-4.606	22.378		58.16
ATOM	5658 5659	CG	LYS	721	39.005	-5.977	22.316		62.49
ATOM	5660	CE	LYS LYS	721	38.449	-6.873	23.401		66.40
ATOM	5661	NZ	LYS	721 721	38.474	-8.329	22.995		68.27
ATOM	5665	C	LYS	721	38.107	-9.194	24.156		75.61
ATOM	5666	0	LYS	721	38.930 37.884	-4.241	19.985		56.00
ATOM	5667	N	PRO	722	40.133	-4.532 -4.439	19.403		59.26
ATOM	5668	CD	PRO	722	41.461	-3.968	19.423		54.10
MOTA	5669	CA	PRO	722	40.208	-5.046	19.836 18.094		53.72
ATOM	5670	СВ	PRO	722	41.702	-4.953	17.759		51.82 49.09
ATOM	5671	CG	PRO	722	42.143	-3.768	18.501		49.09
ATOM	5672	C	PRO	722	39.765	-6.498	18.123		50.10
ATOM	5673	0	PRO	722	39.678	-7.120	19.188		48.82
ATOM	5674	N	SER	723	39.453	-7.020	16.945		49.87
ATOM	5676	CA	SER	723	39.079	-B.410	16.814		50.27
ATOM	5677	СВ	SER	723	38.396	-8.643	15.473	1.00	
MOTA	5678	OG	SER	723	39.273	-8.323	14.404	1.00	
ATOM	5680	С	SER	723	40.414	-9.144	16.872	1.00	
ATOM	5681	0	SER	723	41.400	-8.679	16.311	1.00	
ATOM	5682	N	ASN	724	40.445		17.551	1.00	
ATOM	5684	CA	ASN	724	41.673		17.706	1.00	
ATOM	5685	СВ	ASN	724		-11.286	16.359	1.00	
ATOM	5686	CG	ASN	724		-12.345	15.543	1.00	
ATOM	5687	OD1		724		-13.508	15.948	1.00	
							,		5 50

ATOM	5688	ND2	. ASN	724	41.154	-11.960	14.403	1.00 60.12
ATOM	5691	С	ASN	724	42.622	-10.381	18.683	1.00 57.26
MOTA	5692	0	ASN	724	43.786	-10.131	18.383	1.00 58.40
MOTA	5693	N	CYS	725	42.089	-10.045	19.845	1.00 57.58
MOTA	5695	CA	CYS	725	42.852	-9.418	20.908	1.00 57.02
MOTA	5696	CB	CYS	725	42.835	-7.885	20.803	1.00 55.65
ATOM	5697	SG	CYS	725	43.782	-7.034	22.119	1.00 52.17
ATOM	5698	С	CYS	725	42.158	-9.884	22.177	1.00 56.53
ATOM	5699	0	CYS	725	40.927	-9.954	22.240	1.00 55.99
MOTA	5700	N	THR	726	42.957	-10.279	23.155	1.00 56.09
ATOM	5702	CA	THR	726	42.453	-10.773	24.423	1.00 57.09
ATOM	5703	CB	THR	726	43.551	-11.579	25.129	1.00 57.12
ATOM	5704	OG1	THR	726	44 588	-10.696	25.562	1.00 59.14
MOTA	5706	CG2	THR	726	44.152	-12.587	24.154	1.00 55.09
ATOM	5707	C	THR	726	41.994	-9.608	25.288	1.00 57.58
ATOM	5708	0	THR	726	42.555	-8.518	25.195	1.00 58.49
ATOM	5709	Ň	ASN	727	40.979	-9.832	26.120	1.00 58.48
ATOM	5711	CA	ASN	727	40.482	-8.774	26.986	1.00 58.74
MOTA	5712	CB	ASN	727	39.331	-9.267	27.864	1.00 66.81
ATOM	5713	C.G	ASN	727	39.674	-10.534	28.631	1.00 76.72
ATOM	5714	OD1	ASN	727	40.778	-10.689	29.161	1.00 80.48
ATOM	5715	ND2	ASN	727	38.716	-11.458	28.689	1.00 82.39
ATOM	5718	C	ASN	727	41.606	8.238	27.852	1.00 55.48
ATOM	5719	0	ASN	727	41.589	-7.080	28.255	1.00 51.24
MOTA	5720	N	GLU	728	42.589	-9.099	28.114	1.00 55.37
ATOM	5722	CA	GLU	728	43.757	-8.739	28.913	1.00 55.53
ATOM	5723	CB	GLU	728	44.611	-9.983	29.198	1.00 55.75
ATOM	5724	CG	GLU	728	45.881	-9.699	30.006	1.00 58.24
ATOM	5725	CD	GLU	728	46.606	-10.958	30.463	1.00 58.16
ATOM	5726		GLU	728	46.977	-11.796	29.611	1.00 56.39
ATOM	5727		GLU	728	46.816	-11.102	31.686	1.00 58.35
MOTA	5728	C	GLU	728	44.564	-7.685	28.153	1.00 54.11
ATOM	5729	9	GLU	728	44.790	-6.575	28.654	1.00 55.67
ATOM	5730	N	LEU	729	44.954	-8.020	26.926	1.00 49.65
ATOM	5732	CA	LEU	729	45.715	-7.106	26.086	1.00 46.10
ATOM	5733	CB	LEU	729	46.038	-7.766	24.742	1.00 39.77
ATOM	5734	CG	LEU	729	47.136	-8.836	24.848	1.00 36.12
ATOM	5735		LEU	729	47.118	-9.757	23.673	1.00 34.89
ATOM	5736		LEU	729	48.498	-8.193	24.987	1.00 33.47
ATOM	5737	C	LEU	729	44.950	-5.794	25.908	1.00 45.05
ATOM	5738	0	LEU	729	45.522	-4.713	26.019	1.00 45.58
ATOM	5739	N	TYR	730	43.640	-5.884	25.722	1.00 43.53
ATOM	5741 5742	CA	TYR	730	42.831	-4.692	25.557	1.00 43.57
ATOM		CB	TYR	730	41.414	-5.064	25.097	1.00 41.49
ATOM	5743 5744	CG	TYR	730	40.492	-3.870	24.951	1.00 40.28
ATOM		CD1		730 730	40.763	-2.865	24.013	1.00 36.86
ATOM	5745	CE1		730	39.937	-1.752	23.891	1.00 36.21
	5746	CD2		730	39.361	-3.730	25.768	1.00 39.44
ATOM ATOM	5747		TYR	730	38.522	-2.616	25.654	1.00 38.13
ATOM	5748	CZ	TYR	730	38.817	-1.632	24.712	1.00 38.79
ATOM	5749	OH	TYR	730	37.974	-0.542	24.575	1.00 40.32
MIUM	5751	С	TYR	730	42.806	-3.866	26.856	1.00 44.45

MOTA	5752	0	TYR	730	42.786	-2.632	26.818	1.00 43.45
ATOM	5753	N	MET	731	42.798	-4.534	28.006	1.00 46.44
MOTA	5755	CA	MET	731	42.805	-3.812	29.279	1.00 48.59
ATOM	5756	CB	MET	731	42.516	-4.748	30.447	1.00 54.69
MOTA	5757	CG	MET	731	41.132	-5.387	30.398	1.00 62.68
MOTA	5758	SD	MET	731	39.781	-4.189	30.392	1.00 70.49
MOTA	5759	CE	MET	731	39.492	-4.012	32.209	1.00 72.27
ATOM	5760	С	MET	731	44.167	-3.139	29.450	1.00 46.48
MOTA	5761	0	MET	731	44.280	-2.085	30.086	1.00 44.91
MOTA	5762	N	MET	732	45.202	-3.751	28.881	1.00 43.80
ATOM	5764	CA	MET	732	46.538	-3.167	28.939	1.00 43.03
MOTA	5765	CB	MET	732	47.593	-4.104	28.322	1.00 39.44
ATOM	.5766-	. CG.	MET	732	49.028	-3.578	28.427	1.00 36.02
MOTA	5767	SD	MET	732	50.312	-4.775	27.979	1.00 36.47
ATOM	5768	CE	MET	732	50.547	-5 573	29.530	1.00 41.29
MOTA	5769	С	MET	732	46 474	-1.833	28.188	1.00 42.08
ATOM	5770	0	MET	732	46.995	-0.827	28.659	1.00 42.14
MOTA	5771	N	MET	733	45.775	-1.822	27.054	1.00 43.14
MOTA	5773	CA	MET	733	45.608	-0.609	26.257	1.00 42.24
ATOM	5774	CB	MET	733	44.852	-0.877	24.947	1.00 41.41
ATOM	5775	CG	MET	733	45.607	-1.730	23.938	1.00 40.23
ATOM	5776	SD	MET	733	44.669	-2.025	22.419	1.00 38.02
ATOM	5777	CE	MET	733	45.183	-3.724	21.982	1.00 28.12
ATOM	5778		MET	733	44.820	0.392	27.074	1.00 41.68
MOTA	5779	0	MET	733	45.215	1.550	27.196	1.00 43.78
ATOM	5780	N	ARG	734	43.713	-0.053	27.655	1.00 42.59
ATOM	5782	CA	ARG	734	42.893	0.839	28.467	1.00 42.92
ATOM	5783	CB	ARG	734	41.642	0.119	28.966	1.60 42.35
MOTA	5784	CG	ARG	734	40.753	-0.374	27.852	1.00 39.76
ATOM	5785	CD	ARG	734	40.360	0.763	2€.959	1.00 41.83
ATOM	5786	NE	ARG	734	39.535	1.745	27.653	1.00 45.3€
ATOM	5788	CZ	ARG	734	38.207	1.693	27.708	1.00 50.22
ATOM	5789		ARG	734	37.542	0.708	27.117	1.00 51.18
ATOM	5792	NH2	ARG	734	37.534	2.642	28.346	1.00 53.24
ATOM ATOM	5795	C	ARG	734	43.719	1.385	29.630	1.00 42.42
ATOM	5796 5797	И	ARG	734	43.610	2.571	29.969	1.00 42.59
ATOM	5799	CA	ASP ASP	735	44.591	0.544	30.187	1.00 41.40
ATOM	5800	CB	ASP	735 735	45.464	0.959	31.286	1.00 43.33
ATOM	5801	CG	ASP	735 735	46.337	-0.194	31.755	1.00 48.28
ATOM					45.556	-1.256	32.496	1.00 54.86
ATOM	5802 5803		ASP ASP	735 735	45.903	-2.451	32.322	1.00 53.49
ATOM	5804	C	ASP		44.612	-0.900	33.245	1.00 55.59
ATOM	5805	0	ASP	735 735	46.365	2.107	30.840	1.00 42.65
ATOM	5806	N	CYS	736	46.484	3.124	31.543	1.00 44.03
ATOM	5808	CA	CYS	736	47.021 47.896	1.926 2.952	29.693	1.00 38.83
ATOM	5809	CB	CYS	736	48.545		29.140	1.00 35.90
ATOM	5810	SG	CYS	736	49.634	2.468	27.858	1.00 33.62
ATOM	5811	C	CYS	736		1.087	28.104	1.00 33.92
ATOM	5812	0	CYS	736 736	47.100 47.651	4.208	28.855	1.00 35.96
ATOM	5813	N	TRP	737		5.309	28.830	1.00 35.59
ATOM	5815	CA	TRP	737 737	45.793	4.039	28.668	1.00 38.02
ALON	2012	CA	IRP	131	44.906	5.156	28.372	1.00 40.14

ATOM	5816	CB	TRP	737	43.910	4.766	27.274	1.00 40.93
ATOM	5817	CG	TRP	7 37	44.563	4.379	25.977	1.00 42.36
ATOM	5818	CD2	TRP	737	44.018	3.518	24.969	1.00 43.84
ATOM	5819	CE2	TRP	737	44.972	3.437	23.929	1.00 46.42
MOTA	5820	CE3	TRP	737	42.817	2.806	24.845	1.00 42.43
MOTA	5821	CD1	TRP	737	45.793	4.775	25.519	1.00 42.57
ATOM	5822	NE1	TRP	737	46.043	4.214	24.292	1.00 44.22
MOTA	5824	CZ2	TRP	737	44.756	2.666	22.773	1.00 44.97
ATOM	5825	CZ3	TRP	737	42.606	2.042	23.699	1.00 40.74
MOTA	5826	CH2	TRP	737	43.571	1.978	22.682	1.00 40.75
MOTA	5827	C	TRP	737	44.157	5.706	29.584	1.00 40.62
ATOM	5828	0	TRP	737	43.085	6.285	29.437	1.00 41.37
ATOM	5829	N	HIS	73.8	44.706	5.533	30.783	1.00 42.09
ATOM	5831	C:A	HIS	738	44.044	6.059	31.966	1.00 43.78
MOTA	5832	CB	HIS	738	44.635	5.463	33.248	1.00 46.52
MOTA	5833	CG	HIS	738	43.878	5.844	34.486	1.00 52.24
MOTA	5834	CD3	HIS	738	43.599	7.053	35.025	1.00 50.95
MOT.4	5835	ND1	HIS	738	43.271	4.914	35.299	1.00 56.16
MOTA	5837		HIS	738	42.643	5.536	36.285	1.00 57.23
MOTA	5838	NE2	HIS	73B	42.827	6.835	36.141	1.00 53.22
MOTA	5840	C	HIS	738	44.183	7.577	31.964	1.00 42.81
ATOM	5841	0	HIS	738	45.235	8.093	31.654	1.00 42.12
MOTA	5842	N	ALA	739	43.121	8.285	32.324	1.00 45.66
ATOM	5844	CA	ALA	739 .	43.130	9.750	32.350	1.00 49.42
ATOM	5845	CB	ALA	739	41.739	10.262	32.681	1.00 53.04
ATOM	5846	C	ALA	739	44.167	10.380	33.291	1.00 50.18
ATOM	5847	O	ALA	739	44.710	11.450	33.006	1.00 51.86
MOTA	5848	N	VAL	740	44.322	9.780	34.466	1.00 49.96
ATOM	5850	CA	VAL	740	45.299	10.219	35.467	1.00 50.17
ATOM	5851	CB	VAL	740	44.828	9.849	36.881	1.00 50.33
ATOM	5852		VAL	740	45.880	10.209	37.896	1.00 51.40
ATOM	5853	CG2	VAL	740	43.534	10.559	37.193	1.00 50.86
ATOM	5854	С	VAL	740	46.626	9.497	35.196	1.00 49.81
ATOM	5855	0	VAL	740	46.749	8.295	35.472	1.00 49.85
MOTA	5856	Ŋ	PRO	741	47.646	10.230	34.713	1.00 47.92
ATOM	5857	CD	PRO	741	47.618	11.683	34.476	1.00 46.97
ATOM	5858	CA	PRO	741	48.968	9.686	34.393	1.00 46.47
ATOM	5859	CB	PRO	741	49.796	10.941	34.134	1.00 44.38
MOTA	5860	CG	PRO	741	48.800	11.877	33.561	1.00 44.86
ATOM	5861	C	PRO	741	49.593	8.815	35.480	1.00 47.21
ATOM	5862	0	PRO	741	50.243	7.816	35.176	1.00 46.77
MOTA	5863	N	SER	742	49.380	9.181	36.741	1.00 48.87
ATOM	5865	CA	SER	742	49.939	8.430	37.860	1.00 50.19
ATOM	5866 5067	CB	SER	742	49.753	9.203	39.166	1.00 51.87
ATOM	5867	OG	SER	742	48.389	9.514	39.391	1.00 54.19
ATOM	5869 5870	C	SER	742	49.331	7.040	38.010	1.00 51.30
ATOM	5870	0	SER	742	49.863	6.192	38.723	1.00 51.14
ATOM	5871	N	GLN	743	48.207	6.814	37.343	1.00 53.07
ATOM	5873	CA	GLN	743	47.531	5.531	37.414	1.00 53.50
ATOM	5874	CB	GLN	743	46.015	5.745	37.548	1.00 59.34
ATOM	5875	CG	GLN	743	45.412	5.307	38.898	1.00 66.19
ATOM	5876	CD	GLN	743	46.133	5.896	40.106	1.00 70.07

MOTA	5877	OE1	GLN	743	46.750	5.170	40.885	1.00 73.86
ATOM	5878	NE2	GLN	743	46.047	7.209	40.273	1.00 72.01
ATOM	5881	С	GLN	743	47.850	4.613	36.236	1.00 51.14
ATOM	5882	0	GLN	743	47.504	3.425	36.266	1.00 51.79
MOTA	5883	N	ARG	744	48.484	5.153	35.196	1.00 48.31
MOTA	5885	CA	ARG	744	48.849	4.343	34.027	1.00 45.49
ATOM	5886	CB	ARG	744	49.326	5.224	32.869	1.00 40.33
ATOM	5887	CG	ARG	744	48.322	6.200	32.324	1.00 36.32
MOTA	5888	CD	ARG	744	48.944	7.100	31.262	1.00 28.55
MOTA	5889	NE	ARG	744	48.050	8.203	30.961	1.00 28.86
ATOM	5891	CZ	ARG	744	48.429	9.409	30.547	1.00 30.58
MOTA	5892		ARG	744	49.707	9.700	30.357	1.00 26.02
ATOM	5895	NH2	ARG	744	-47.516	10.354	30.386	1.00 30.62
ATOM	5898	C	ARG	744	50.016	3.454	34.452	1.00 47.35
ATOM	5899	O	ARG	744	50.794	3.824	35.334	1.00 52.01
MOTA	5900	N	PRO	745	50.133	2.251	33.869	1 00 46.36
ATOM	5901	CD	PRO	74'5	49.248	1.559	32.921	1.00 45.54
ATOM	5902	CA	PRO	745	51.261	1:402	34.271	1.00 43.41
ATOM	5903	СВ	PRO	745	50.972	0.078	33.547	1.00 41.77
ATOM	5904	CG	PRO	745	50.155	0.491	32.354	1.00 42.26
MOTA	5905	C	PRO	745	52.590	2.007	33.822	1.00 40.30
ATOM	5906	C	PRO	745	52.621	2.905	32.990	1.00 39.73
ATOM	5907	Ņ	THR	746	53.679	1.570	34.433	1.00 39.14
	5909	CA	THR	746	54.997	2.056	34.039	1.00 38.35
ATOM	5910	CB	THR	746	55.992	2.104	35.249	1.00 36.75
ATOM	5911	OGI	THR	746	56.202	0.776	35.769	1.00 32.25
MOTA	5913	CG2	THR	746	55.47 7	3.037	36.341	1.00 30.31
MOTA	5914	C	THR	746	55. 56 8	1.162	32.987	1.00 37.90
ATOM	5915	0	THR	746	55.185	-0.068	32.938	1.00 37.99
MOTA	5916	N	PHE	747	56.490 .	1.584	32.157	1.00 35.94
ATOM	5918	CA	PHE	747	57.106	0.716	31.161	1.00 35.00
ATOM	5919	CB	PHE	747	58.124	1.469	30.309	1.00 30.45
ATOM	5920	CG	PHE	747	57.512	2.174	29.142	1.00 27.61
ATOM	5921	CD1		747	56.950	1.450	28.103	1.00 23.68
ATOM	5922	CD2		747	57.468	3.558	29.094	1.00 27.97
MOTA	5923	CE1	PHE	747	56.352	2.088	27.033	1.00 23.56
ATOM	5924		PHE	747	56.869	4.209	28.027	1.00 26.92
ATOM ATOM	5925	CZ	PHE	747	56.312	3.470	26.995	1.00 26.21
ATOM	5926	C O	PHE	747	57.766	-0.477	31.826	1.00 36.37
	5927		PHE	747	57.920	-1.525	31.219	1.00 37.11
ATOM	5928	N	LYS	748	58.177	-0.312	33.075	1.00 39.68
ATOM	5930	CA	LYS	748	58.797	-1.411	33.807	1.00 42.20
	5931	CB	LYS	748	59.433	-0.895	35.095	1.00 46.17
ATOM ATOM	5932	CG	LYS	748	59.978	-1.991	35.984	1.00 54.78
	5933	CD	LYS	748	60.794	-1.428	37.135	1.00 58.53
MOTA MOTA	5934	CE	LYS	748	61.239	-2.537	38.075	1.00 59.33
ATOM	5935	NZ	LYS	748	62.167	-2.025	39.120	1.00 62.36
	5939	C	LYS	748	57.723	-2.463	34.111	1.00 42.78
ATOM	5940	0	LYS	748	57.998	-3.664	34.075	1.00 37.97
MOTA	5941	N	GLN	749	56.503	-1.992	34.392	1.00 43.27
MOTA	5943	CA	GLN	749	55.365	-2.866	34.671	1.00 43.39
MOTA	5944	CB	GLN	749	54.146	-2.056	35.146	1.00 47.37

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MOTA	5945	CG	GLN	749	54.236	-1.504	36.569	1.00 51.86
MOTA	5946	CD	GLN	749	53.036	-0.639	36.938	1.00 54.76
ATOM	5947	OE1	. GLN	749	53.181	0.504	37.350	1.00 58.36
ATOM	5948	NE2	GLN	749	51.846	-1.179	36.769	1.00 59.25
ATOM	5951	С	GLN	749	55.006	-3.607	33.389	1.00 41.66
MOTA	5952	0	GLN	749	54.978	-4.841	33.355	1.00 40.25
ATOM	5953	N	LEU	750	54.759	-2.843	32.327	1.00 41.47
ATOM	5955	CA	LEU	750	54.398	-3.387	31.018	1.00 40.00
ATOM	5956	CB	LEU	750	54.366	-2.279	29.966	1.00 40.55
ATOM	5957	CG	LEU	750	53.316	-1.174	30.112	1.00 39.94
ATOM	5958	CD1	LEU	750	53.714	0.019	29.257	1.00 41.03
MOTA	5959	CD2	LEU	750	51.952	-1.696	29.722	1.00 37.80
ATOM	5960	С	LEU	.750	55.383	-4.452	30.581	1.00 39.61
MOTA	5961	0	LEU	750	54.990	-5.470	30.027	1.00 42.08
ATOM	5962	N	VAL	751	56.670	-4.207	30.804	1.00 40.63
ATOM	5964	CA	VAL	751	57.691	-5.177	30.422	1.00 39.65
MOTA	5965	СВ	VAL	751	59.115	-4.639	30.677	1.00 33.44
ATOM	5966	CG1	VAL	751	60.142	-5.694	30.351	1.00 31.57
ATOM	5967	CG2	VAL	751	59.372	-3.433	29.825	1.00 25.19
ATOM	5968	C	VAL	751	57.458	-6.468	31.204	1.00 43.58
ATOM	5969	0	VAL	751	57.530	-7.563	30.646	1.00 44.81
ATOM	5970	N	GLU	752	57.116	- 6 339	32.481	1.00 46.24
ATOM	5972	CA	GLU	752	56.869	-7.518	33.301	1.00 50.55
MOTA	5973	CB	GLU	752	56.781	-7.137	34.783	1.00 53.70
ATOM	5974	CG	GLU	752	58.090	-6.541	35.310	1.00 56.60
MOTA	5975	CD	GLU	752	58.079	-6.243	36.792	1.00 56.20
ATOM	5976	OE1	GLU	752	58.387	-5.092	37.178	1.00 53.45
MOTA	5977	OE2	GLU	752	57.789	-7.170	37.573	1.00 60.28
ATOM	5978	C	GLU	752	55.622	-8.275	32.837	1.00 50.90
MOTA	5979	o	GLU	752	55.689	-9.474	32.555	1.00 51.03
ATOM	5 9 80	N	ASP	753	54.501	-7.570	32.708	1.00 51.12
MOTA	5982	CA	ASP	753	53.251	-8.184	32.265	1.00 48.76
ATOM	5983	CB	ASP	753	52.122	-7.160	32.249	1.00 51.11
ATOM	5984	CG	ASP	753	51.646	-6.805	33.636	1.00 54.97
ATOM	5985	OD1	ASP	753	51.592	-7.715	34.495	1.00 58.37
ATOM	5986	OD2	ASP	753	51.319	-5.618	33.864	1.00 56.38
ATOM	5987	C	ASP	753	53.381	-8.790	30.881	1.00 48.02
MOTA	5988	0	ASP	753	52.991	-9.935	30.672	1.00 48.32
MOTA	5989	N	LEU	754	53.925	-8.020	29.940	1.00 45.16
ATOM	5991	CA	LEU	754	54.111	-8.490	28.571	1.00 44.82
MOTA	5992	CB	LEU	754	54.696	-7.387	27.691	1.00 42.70
ATOM	5993	CG	LEU	754	53.736	-6.263	27.298	1.00 42.92
ATOM	5994	CD1	LEU	754	54.500	-5.236	26.495	1.00 41.44
ATOM	5995	CD2	LEU	754	52.537	-6.822	26.502	1.00 42.86
MOTA	5996	C	LEU	754	55.001	-9.716	28.529	1.00 46.00
ATOM	5997	0	LEU	754	54.815	-10.606	27.708	1.00 45.88
MOTA	5998	N	ASP	755	55.975	-9.752	29.424	1.00 47.37
MOTA	6000	CA	ASP	755	56.889	-10.873	29.516	1.00 48.88
MOTA	6001	CB	ASP	755	57.898	-10.584	30.628	1.00 49.89
ATOM	6002	CG	ASP	755	58.998	-11.616	30.717	1.00 51.73
MOTA	6003	OD1	ASP	755	59.640	-11.680	31.785	1.00 55.47
ATOM	6004	OD2	ASP	755	59.236	-12.354	29.738	1.00 50.98

ATOM	6005	С	ASP	755	56.024 -12.093	29.864	1.00 51.26
MOTA	6006	0	ASP	7 55	56.021 -13.107	29.155	1.00 50.49
ATOM	6007	N	ARG	756	55.227 ~11.940	30.917	1.00 52.15
MOTA	6009	CA	ARG	756	54.332 -12.989	31.385	1.00 53.30
MOTA	6010	CB	ARG	756	53.556 -12.501	32.611	1.00 54.54
MOTA	6011	CG	ARG	756	52.389 -13.380	33.029	1.00 54.26
MOTA	6012	CD	ARG	756	51.672 -12.772	34.215	1.00 56.76
MOTA	6013	NE	ARG	756	51.293 -11.382	33.969	1.00 61.39
MOTA	6015	CZ	ARG	756	50.259 -11.002	33.221	1.00 62.60
MOTA	6016	NH1	ARG	756	49.487 -11.909	32.642	1.00 61.18
ATOM	6019	NH2	ARG	756	49.986 -9.711	33.064	1.00 63.72
ATOM	6022	C	ARG	756	53.357 -13.420	30.297	1.00 53.03
ATOM	6023	0	ARG	756	. 53.243 -14.607	30000	1:00 54.82
MOTA	6024	N	ILE	757	52.687 -12.452	29.680	1.00 51.18
ATOM	6026	CA	ILE	757	51.709 -12.732	28.630	1.00 48.68
ATOM	6027	CB	ILE	757	51.025 -11.435	28.120	1.00 47.88
ATOM	6028	CG2	ILE	757	50.112 -11.752	26.953	1.00 45.56
MOTA	6029	CG1	ILE	757	50.247 -10.763	29.258	1.00 47.77
ATOM	6030	CD1	ILE	757	49.651 -9.414	28.914	1.00 46.00
MOTA	6031	С	ILE	757	52.314 -13.482	27.449	1.00 48.30
ATOM	6032	0	ILE	757	51.694 -14.409	26.937	1.00 45.61
ATOM	6033	N	VAL	758	53.523 -13.094	27.038	1.00 48 88
MOTA	6035	CA	VAL	758	54.202 - 7.3.734	25.912	1.00 49.96
ATOM	6036	CB	VAL	758	55.602 -13 101	25.615	1.00 47.80
ATOM	6037	CG1	VAL	758	56.313 -13.864	24.502	1.00 44.17
ATOM	6038	CG2	VAL	758	55.461 -11.660	25.188	1.00 46.65
ATOM	6039	С	VAL	758	54.378 -15.217	26.196	1.00 54.00
MOTA	6040	0	VAL	758	54.218 ~16.050	25.306	1.00 53.52
ATOM	6041	N	ALA	759	54.697 -15.540	27.445	1.69 57.83
ATOM	6043	CA	ALA	759 .	54.898 -16.926	27.844	1.00 61.94
ATOM	6044	CB	ALA	759	55.447 -16.987	29.257	1.00 62.30
ATOM	6045	С	ALA	759	53.592 -17.702	27.761	1.00 65.09
ATOM	6046	0	ALA	759	53.555 -18.823	27.254	1.00 66.39
ATOM	6047	N	LEU	760	52.519 -17.090	28.248	1.00 66.99
ATOM	6049	CA	LEU	760	51.209 -17.720	28.246	1.00 68.78
ATOM	6050	CB	LEU	760	50.314 -17.090	29.320	1.00 68.07
ATOM	6051	CG	LEU	760	50.729 -17.330	30.777	1.00 67.01
ATOM	6052		LEU	760	49.808 -16.563	31.722	1.00 67.93
ATOM	6053		LEU	760	50.701 -18.819	31.083	1.00 65.17
ATOM	6054	С	LEU	760	50.510 -17.666	26.892	1.00 71.19
ATOM	6055	0	LEU	760	49.342 -18.039	26.787	1.00 73.15
ATOM	6056	N	THR	761	51.210 -17.201	25.860	1.00 73.38
ATOM	6058	CA	THR	761	50.626 -17.113	24.518	1.00 73.92
MOTA	6059	CB	THR	761	50.963 -15.760	23.829	1.00 72.65
ATOM	6060		THR	761	50.353 -14.690	24.555	1.00 74.44
ATOM	6062	CG2		761	50.435 ~15.731	22.420	1.00 70.32
ATOM	6063	С	THR	761	51.080 -18.276	23.636	1.00 74.66
ATOM	6064	0	THR	761	52.276 -18.520	23.463	1.00 75.08
ATOM	6065	SG	CYS	1603	19.100 -9.073	19.903	0.50 30.84 PRT2
ATOM	6066	CG	MET	534	69.385 12.295	23.393	0.50 33.69 PRT2
ATOM	6067	SD	MET	534	69.112 13.312	24.832	0.50 34.44 PRT2
ATOM	6068	CE	MET	534	70.067 12.429	26.060	0.50 36.92 PRT2

ATOM	6069	SG CYS	603	56.370	-7.959	16.451	0.50 41.20	PRT2
MOTA	2716	OH2 TIP3	1	71.864	25.128	2.721	1.00 26.20	
MOTA	2719	OH2 TIP3	2	39.862	4.160	16.115	1.00 42.43	
MOTA	2722	OH2 TIP3	3	83.875	19.969	10.572	1.00 23.41	
MOTA	2725	OH2 TIP3	4	83.585	20.356	7.953	1.00 30.15	
MOTA	2728	OH2 TIP3	5	75.100	16.407	6.948	1.00 46.78	
MOTA	2731	OH2 TIP3	6	86.616	19.701	9.707	1.00 44.37	
MOTA	2734	OH2 TIP3	7	52.270	10.726	24.472	1.00 40.13	
ATOM	2737	OH2 TIP3	8	55.346	9.394	22.489	1.00 29.09	
ATOM	2740	OH2 TIP3	9	56.794	4.380	32.527	1.00 28.02	
MOTA	2743	OH2 TIP3	10	52.425	4.653	13.421	1.00 18.63	
ATOM	2746	OH2 TIP3	11	41.527	5.347	22.682	1.00 32.60	
ATOM	. 2749	OH2 TIP3	12	44.868	9.058	21.659	1,.00 34.90	
ATOM	2752	OH2 TIP3	13	64.548	-2.881	29.048	1.00 32.56	
MOTA	2755	OH2 TIP3	14	77.179	13.205	23.892	1.00 30.36	
MOTA	2758	OH2 TIP3	15	79.309	16.826	18.132	1.00 55.69	
ATOM	2761	OH2 TIP3	16	83.279	11.681	16.069	1.00 21.18	
MOTA	2764	OH2 TIP3	17	13.978	-9.614	0.374	1.00 23.81	
ATOM:	2767	OH2 TIP3	18	38.294	0.616	5.237	1.00 48.89	
MOTA	2770	OH2 TIP3	19	27.114	6.248	5.051	1.00 19.82	
MOTA	2773	OH2 TIP3	20	34.369	-1.759	16.798	1.00 43.83	
MOTA	2776	OH2 TIP3	21	20.500	2.296	28.237	1.00 53.46	
ATOM	2779	OH2 TIP3	22	50.938	-11.733	38.257	1.00 51.73	
MOTA	2782	OH2 TIP3	23	17.066	-5.917	-2.027	1.00 29 88	
ATOM	2785	OH2 TIP3	24	27.873	8.078	15.136	1.00 45.40	
MOTA	2788	OH2 TIP3	25	31.459	0.037	6.873	1.00 33.38	
MOTA	2791	OH2 TIP3	26	27.088	-12.845	27.724	1.00 37.01	
MOTA	2794	OH2 TIP3	27	28.577	-17.329	12.884	1.00 37.31	
MOTA	2797	OH2 TIP3	28	88.863	14.111	8.054	1.06 41.25	
ATOM	2800	OH2 TIP3	29	-2.311	-3.712	11.489	1.00 30.72	
ATOM	2803	OH2 TIP3	30	34.895	·4.269	18.658	1.00 28.99	
MOTA	2806	OH2 TIP3	31	80.531	18.007	9.739	1.00 23.83	
ATOM	2809	OH2 TIP3	32	5.519	3.787	10.528	1.00 20.39	
ATOM	2812	OH2 TIP3	33	-10.523	5.304	11.469	1.00 20.31	
ATOM	2815	OH2 TIP3	34	29.538	-8.848	20.187	1.00 43.26	
ATOM	2818	OH2 TIP3	35	5.866	3.469	13.367	1.00 21.16	
ATOM	2821	OH2 TIP3	36	31.810	3.038	0.203	1.00 65.03	
ATOM	2824	OH2 TIP3	37	19.879	2.087	-3.828	1.00 34.62	
ATOM	2827	OH2 TIP3	38	61.882	2.577	32.790	1.00 43.01	
MOTA	2830	OH2 TIP3	39	21.062	-6.897	-4.255	1.00 26.18	
ATOM	2833	OH2 TIP3	40	-15.562	8.847	22.744	1.00 40.33	
ATOM	2836	OH2 TIP3	41	40.043	2.380	8.610	1.00 65.14	
ATOM	2839	OH2 TIP3	42	19.176	11.322	0.332	1.00 33.04	
ATOM	2842	OH2 TIP3	43	67.221	8.965	17.535	1.00 14.78	
MOTA	2845	OH2 TIP3	44	87.877	18.828	18.789	1.00 50.00	
MOTA	2848	OH2 TIP3	45	74.676	17.083	4.253	1.00 43.45	
ATOM	2851	OH2 TIP3	46	29.458	16.709	10.527	1.00 37.44	
MOTA	2854	OH2 TIP3	47	66.590	7.242	15.359	1.00 27.63	
MOTA	2857	OH2 TIP3	48	85.038	21.651	5.881	1.00 27.12	
ATOM	2860	OH2 TIP3	49	-4.762	3.091	3.313	1.00 13.83	
MOTA	2863	OH2 TIP3	50	19.509	4.951	5.063	1.00 33.74	
ATOM	2866	OH2 TIP3	51	34.833	5.465	24.635	1.00 32.77	

MOTA	2869	OH2	TIP3	52	34.907	-17.187	13.739	1.00	39.47	
ATOM	2872	OH2	TIP3	53	60.000	7.568	27.982		31.38	
ATOM	2875	OH2	TIP3	54	-7.341	-1.418	6.308		40.22	
MOTA	2878	OH2	TIP3	55	55.21B	12.161	25.430		40.99	
ATOM	2881	OH2	TIP3	56	68.597	6.912	16.955		45.39	
ATOM	2884	OH2	TIP3	57	73.486	20.957	19.260		49.23	
MOTA	2887	OH2	TIP3	58	3.555	-8.367	-8.166		20.02	•
MOTA	2890	OH2	TIP3	59	38.079	10.933	5.669		27.07	
MOTA	2893	OH2	TIP3	60	29.817	-9.690	-1.649		44.28	
ATOM	2896	OH2	TIP3	61	49.332	1.501	12.262		42.78	
ATOM	2899	ОН2	TIP3	62	41.366	3969	28.834		37.60	
MOTA	2902	OH2	TIP3	63	10.523	-13.468	0.864		45.18	
MOTA	2905	OH2	TIP3	64	-1.001	-4.658	21.574		35.58	
MOTA	2908	OH2	TIP3	65	30.278	16.435	13.217		48.75	
ATOM	2911	OH2	TIP3	66	8.115	4.304	3.317	1.00	16.04	
ATOM	2914	OH2	TIP3	67	73.460	18.707	22.744		34.79	
ATOM	2917	OH2	TIP3	68	-8.041	-3.332	24.939	1.00	44.96	
ATOM	2920	OH2	TIP3	69	66.672	-4.643	28.739	1.00	62.39	
ATOM	2923	OH2	TIP3	70	21.770	-20.943	4.990	1.00	32.98	
MOTA	2926	OH2	TIP3	71	59.587	-6.482	5.018	1.00	37.78	
ATOM	2929	OH2	TIP3	72	16.676	-13.158	-3.023	1.00	42.74	
MOTA	2932	OH2	TIP3	73	-15.177	7.529	4.524	1.00	19.90	
ATOM	2935	OH2	TIP3	74	33.105	2.738	13.267	1.00	40.43	
ATOM	2938		TIP3	75	0.334	-2.795	10.999	1.00	31.20	
ATOM	2941		TIP3	76	17.489	2.568	5.445	1.00	16.38	
ATOM	2944		TIP3	77	27.373	3.870	6.168	1.00	39.52	
MOTA	2947		TIP3	78	-8.546	6.378	9.673	1.00	17.89	
ATOM	2950		TIF3	79	1.508	-1.891	8.809	1.00	33.71	
ATOM	2953		TIP3	80	~4.985	-3.C24	6.965	1.00	29.65	
ATOM	2956		TIP3	51	17.673	3.029	1.736	1.00	22.73	
ATOM	2959		TIP3	82	20.319	3.536	2.883	1.00	20.39	
ATOM	2962		TIP3	83	0.366	-2.4)9	22.243		22.15	
ATOM	2965		TIP3	84	19.688	-6.134	-1.678	1.00	13 22	
ATOM	2968		TIP3	85		-15.481	6.681	1.00	43.14	
ATOM	2971		TIP3	86		-12.368	11.861	1.00	38.38	
ATOM ATOM	2974		TIP3	87	6.421	1.053	-3.368		21.50	
ATOM	2977		TIP3	88	-13.766	1.683	5.565		39.45	
ATOM	2980		TIP3	89	15.689	-7.291	-0.140		30.27	
ATOM	2983 2986		TIP3	90	-1.762	-5.389	3.937		31.03	
ATOM	2989		TIP3	91 92	12.642	5.184	-4.424		37.94	
ATOM	2992		TIP3	92	69.601	27.513	2.309		44.71	
ATOM	2995		TIP3	93		-13.465	-0.010		50.74	
ATOM	2998		TIP3	94	60.354	-4.675	33.978		38.15	
ATOM	3001			95	10.408	5.632	3.428		51.37	
ATOM	3001		TIP3	96 97	-9.676	-3.916	4.621		34.12	
ATOM	3004		TIP3	97	73.207	-2.076	10.677		70.04	
ATOM	3007		TIP3	98	-3.042	5.487	30.579		30.78	
ATOM ,	3013		TIP3	99 300	36.627	0.829	11.645		41.40	
MOTA	3016		TIP3	100 101	21.685 31.434	6.318	16.814		20.93	
ATOM	3019		TIP3	101		0.662	19.231		57.99	
MOTA	3022		TIP3		5.793	-8.713	22.177		54.77	
LI OU	3022	UH2	11173	103	-13.037	8.412	17.695	1.00	25.61	

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MOTA 3025 OH2 TIP3 104 26.597 -10.647 -1.184 1.00 25.85 MOTA 3028 OH2 TIP3 105 24.406 1.951 18.037 1.00 30.72 **ATOM** 3031 OH2 TIP3 106 -1.809 12.914 3.754 1.00 43.57 **ATOM** 3034 OH2 TIP3 107 59.590 13.738 33.131 1.00 26.96 MOTA 3037 OH2 TIP3 108 4.442 -11.011 1.724 1.00 46.96 MOTA 3040 OH2 TIP3 109 8.101 2.869 0.801 1.00 37.28 **ATOM** 3043 OH2 TIP3 110 76.065 1.631 26.158 1.00 46.49 48.821 15.839 **ATOM** 3046 OH2 TIP3 111 14.239 1.00 34.18 ATOM 3049 OH2 TIP3 2.703 -11.324 8.959 1.00 39.16 112 ATOM 3052 OH2 TIP3 113 82.922 26.478 12.953 1.00 43.77 ATOM 3055 OH2 TIP3 114 8.998 -6.359 -3.309 1.00 39.51 OH2 TIP3 ATOM 3058 115 -8.590 4.563 4.397 1.00 32.53 MOTA 3061 OH2 TIP3....116 .. 8.115 -13.800 8.351 1.00 41.64 3064 **ATOM** OH2 TIP3 51.643 6.187 10.821 117 1.00 31.70 ATOM 3067 OH2 TIP3 20.737 3.915 15.522 118 1.00 17.40 MOTA 3070 OH2 TIP3 119 73.254 3.698 20.947 1.00 27.49 MOTA 3073 OH2 TIP3 120 5.343 -11.780 22.588 1.00 36.63 **ATOM** 3076 OH2 TIP3 121 34.390 2.307 16.660 1.00 64.04 3079 **ATOM** OH2 TIP3 122 9.552 -11.846 6.934 1.00 28.23 **ATOM** 3082 OH2 TIP3 123 8.463 4.098 -1.454 1.00 30.21 3085 ATOM OH2 TIP3 7.397 6.952 124 2.826 1.00 33.87 ATOM 3088 OH2 TIP3 125 35.796 -1.428 0.072 1.00 30.27 **ATOM** 3091 OH2 TIP3 126 45.044 10.052 11.102 1.00 28.75 **ATOM** 3094 OH2 TIP3 127 45.209 11.756 21.279 1.00 31.80 **ATOM** 3097 OH2 TIP3 128 -2.800 15.170 16.902 1.00 32.72 MOTA 3100 OH2 TIP3 129 85.885 11.248 9.428 1.00 25.28 **ATOM** 3103 OH2 TIP3 130 13.136 -2.420 1.867 1.00 20.56 **ATOM** 3106 OH2 TIP3 131 75.900. 3.542 20.641 1.00 39.79 **ATOM** 3109 OH2 TIP3 13.075 7.580 132 -2.817 1.00 34.49 **ATOM** 3112 OH2 TIP3 133 11.166. -10.189 0.573 1.00 36.71 MOTA 3115 OH2 TIP3 134 13.814 -16.459 3.327 1.00 21.18 MOTA 3118 OH2 TIP3 135 -6.419 -3.460 16.599 1.00 32.62 **MOTA** 3121 OH2 TIP3 136 25.578 -12.834 3.624 1.00 43.32 **ATOM** 3124 OH2 TIP3 -16.472 137 11.136 6.388 1.00 64.77 MOTA 3127 OH2 TIP3 138 86.531 12.711 7.151 1.00 28.72 MOTA 3130 OH2 TIP3 139 -4.665 32.292 1.511 1.00 30.98 **ATOM** 3133 OH2 TIP3 140 7.369 45.116 11.774 1.00 30.59 ATOM OH2 TIP3 3136 81.035 12.317 16.907 141 1.00 41.72 MOTA 3139 OH2 TIP3 142 2.905 -7.019 -2.101 1.00 26.20 MOTA 3142 OH2 TIP3 143 31.895 -6.253 20.885 1.00 36.12 MOTA 3145 OH2 TIP3 144 74.974 -2.640 12.464 1.00 58.90 MOTA OH2 TIP3 3148 145 7.514 6.734 -1.116 1.00 37.81 MOTA 3151 OH2 TIP3 71.606 5.595 146 22.198 1.00 54.82 MOTA 3154 OH2 TIP3 68.337 147 -5.037 8.955 1.00 40.80 MOTA 3157 OH2 TIP3 148 0.191 -9.669 6.903 1.00 47.40 **ATOM** 3160 OH2 TIP3 149 68.043 18.153 10.710 1.00 36.67 MOTA 3163 OH2 TIP3 150 3.644 8.512 4.478 1.00 40.16 **ATOM** 3166 OH2 TIP3 151 52.117 11.302 18.644 1.00 40.22 MOTA OH2 TIP3 3169 -10.220 6.750 4.981 152 1.00 25.00 ATOM 3172 OH2 TIP3 153 76.944 1.425 -0.793 1.00 46.95 MOTA 3175 OH2 TIP3 154 10.053 -11.958 17.014 1.00 38.99 **ATOM** OH2 TIP3 3178 155 34.348 14.128 18.169 1.00 42.98

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ATOM	3181	OH2 TIP3	156	2.472	-8.230	16.629	1.00 39.28
MOTA	3184	OH2 TIP3	157	29.861	1.764	5.993	1.00 36.29
MOTA	3187	OH2 TIP3	158	32.608	-17.351	11.473	1.00 59.48
MOTA	3190	OH2 TIP3	159	42.408	18.047	11.188	1.00 39.61
MOTA	3193	OH2 TIP3	160	88.019	10.498	5.885	1.00 57.85
MOTA	3196	OH2 TIP3	161	70.091	-4.165	25.232	1.00 64.48
ATOM	3199	OH2 TIP3	162	77.332	5.434	24.000	1.00 55.68
ATOM	3202	OH2 TIP3	163	-0.743	-8.232	4.456	1.00 61.30
ATOM	3205	OH2 TIP3	164	34.224	15.617	1.556	1.00 36.76
MOTA	3208	OH2 TIP3	165	-9.619	7.593	7.404	1.00 36.55
ATOM	3211	OH2 TIP3	166	11.725	5.841	7.590	1.00 33.56
ATOM	3214	OH2 TIP3	167	-8.492	14.057	13.866	1.00 43.88
MOTA	3217	OH2 TIP3	168	32.082	3.374	18.430	1.00 50.87
MOTA	3220	OH2 TIP3	169	-8.471	9.925	24.255	1.00 41.24
ATOM	3223	OH2 TIP3	170	-1.100	-6.507	15.528	1.00 31.24
MOTA	3226	OH2 TIP3	171	80.411	0.680	15.823	1.00 49.76
ATOM	3229	OH2 TIP3	172	67.266	20.862	-1.548	1.00 43.71
MOTA	3232	OH2 TIP3	173	-0.460	4.230	1.362	1.00 29.46
ATOM	3235	OH2 TIP3	174	-0.107	6.721	2.716	1.00 34.57
ATOM	3238	OH2 TIP3	175	-0.955	8.958	1.388	1.00 37.76
ATOM	3241	OH2 TIP3	176	-5.269	9.229	2.243	1.00 38.77
ATOM	3244	OH2 TIP3	177	-7.000	10.196	3.928	1.00 55.41
ATOM	3247	OH2 TIP3	178	2.919	7.005	0.987	1.00 46.54
ATOM	3250	OH2 TIP3	179	5.370	10.843	8.420	1.00 36.98
ATOM	3253	OH2 TIP3	180	63.828	12.793	22.770	1.00 63.91
MOTA	3256	OH2 TIP3	181	79.461	0.958	18 507	1.00 47.46
ATOM	3259	OH2 TIP3	182	59.131	-11.907	7.222	1.00 51.47
ATOM	3262	OH2 TIP3	183	14.248	-1.085	-4.437	1.00 43.62
ATOM	3265	OH2 TIP3	184	59.294	2.993	33.283	1.00 56.42
ATOM	3268	OH2 TIP3	185	32.270	13.672	20.001	1.00 47.71
MOTA	3271	OH2 TIP3	186	72.089	16.139	22.904	1.00 49.99
ATOM	3274	OH2 TIP3	187	1.038	-8.592	14.174	1.00 40.01
ATOM	3277	OH2 TIP3	188	-0.484	5.267	30.679	1.00 48.08
ATOM	3280	OH2 TIP3	189	81.532	15.288	17.279	1.00 79.71
ATOM	3283	OH2 TIP3	190	-17.528	3.859	24.112	1.00 56.21
MOTA	3286	OH2 TIP3	191	27.542	10.591	14.666	1.00 53.58
MOTA	3289	OH2 TIP3	192	34.962	4.381	27.739	1.00 60.92
MOTA	3292	OH2 TIP3	193	-3.244	-3.943	8.937	1.00 35.88
ATOM ATOM	3295	OH2 TIP3	194	42.673	7.836	22.289	1.00 37.44
	3298	OH2 TIP3	195	52.865	12.074	22.272	1.00 35.63
ATOM	3301	OH2 TIP3	196	26.791	13.926	19.808	1.00 76.14
ATOM	3304	OH2 TIP3	197	-7.584	9.157	6.269	1.00 44.54
ATOM	3310	OH2 TIP3	198	55.298	15.955	20.455	1.00 50.69
ATOM	3313	OH2 TIP3	199	51.654	19.308	22.767	1.00 53.00
ATOM	3316	OH2 TIP3	200	20.092	7.039	7.056	1.00 32.98
ATOM	3319	OH2 TIP3	201	28.988	1.734	-3.437	1.00 42.52
ATOM	3322	OH2 TIP3	202	26.359	2.749	-4.689	1.00 43.12
ATOM	3325	OH2 TIP3	203	36.827	2.974	18.493	1.00 57.91
ATOM	3328	OH2 TIP3	204		~20.743	13.983	1.00 62.01
ATOM	3331	OH2 TIP3	205		-14.283	6.114	1.00 79.57
ATOM	3334	OH2 TIP3	206	31.396	1.595	-1.941	1.00 53.29
ATOM	3337	OH2 TIP3	207	10.244	-16.264	15.463	1.00 43.25

ATOM	3340	OH2	TIPE	3 208	7.	255	-11.909	5.440	1.00	45.52
ATOM	3343	OH2	TIPE	3 209	-12.	421	14.520	11.103	1.00	56.32
ATOM	3346	OH2	TIPE	3 210	11.	250	9.879	-1.498	1.00	28.34
ATOM	3349	OH2	TIPE	3 211	11.	426	12.574	-1.341	1.00	37.79
ATOM	3352	OH2	TIP3	212	34.	344	13.104	-1.291	1.00	51.83
ATOM	3355	OH2	TIP3	213	31.	230	18.082	8.054	1.00	44.77
MOTA	3358	OH2			37.	062	12.036	-1.875	1.00	53.61
MOTA	3361		TIP3		. 35.	231	3.150	10.692	1.00	60.59
MOTA	3364		TIP3		63.	913	13.371	26.770	1.00	59.44
MOTA	3367		TIP3		36.	511	6.165	15.409	1.00	70.98
ATOM	3370	OH2	TIP3	218	90.	623	4.459	6.671	1.00	52.23
ATOM	3373	OH2			49.	B22	-11.758	10.881	1.00	46.12
ATOM	3376	OH2			60.	367	-10.286	16.662	1.00	68.41
ATOM	3379	OH2		221	17.	954	-21.378	7.048	1.00	68.51
ATOM	3382	OH2			66.3	176	-1.266	30.784	1.00	39.19
ATOM	3385	OH2			75.2	201	19.402	20.800	1.00	43.98
ATOM	3388	OH2			-2.8	395	10.302	3.534	1.00	44.97
ATOM	3391	OH2			6.0	045	-4.015	25.279	1.00	63.74
АТОМ	3394	OH2			36.2	238	5.898	12.819	1.00	32.89
ATOM	3397	OH2	TIP3		-5.5		16.713	14.089	1.00	51.60
MOTA	3400	OH2	TIP3		46.5		-11.931	26.964	1.00	37.76
ATOM	3403	OH2	TIP3		6.4		6.048	13.722	1.00	27.51
ATOM	3406	OH2	TIP3		-3.6		-5.054	20.691		38.16
ATOM	3409	OH2	TIP3		1.8		-3.444	-0.149		54.03
ATOM	3412	OH2	TIP3		86.1		11.480	23.402	1.50	
ATOM	3415	OH2	TIP3		10.5		7.581	5.716		48.45
ATOM	3421		TIP3	234	64.6		-8.130	20.697		69.67
ATOM ATOM	3424 3427	OH2 OH2	TIP3	235	11.3		-17.736	13.500	1.00	54.61
ATOM	3430	OH2	TIP3	236	3.1		-4.782	21.980		57.12
ATOM	3433		TIP3	237 238	72.2		1.006	-1.987		41.40
ATOM	3436		TIP3	239	50.2		-3.179	32.723		74.99
MOTA	3439	OH2		240	58.0 43.5		9.469 20.498	11.776		44.10
ATOM	3442	OH2		241	67.0		16.597	30.344 15.934		43.69
ATOM	3445	OH2		242	87.6		21.694	5.373		45.80 59.39
ATOM	3448	OH2	TIP3	243	71.7		28.586	7.932	1.00	
ATOM	3451	OH2	TIP3	244	25.9		-8.124	27.084		61.12 42.13
ATOM	3454		TIP3	245	-18.3		10.487	12.859		73.36
MOTA	3457	OH2	TIP3	246	30.7		11.410	16.381		39.24
ATOM	3460		TIP3	247	22.6		-16.025	-2.906		63.22
MOTA	4620	С	SUG	1000	67.8		4.441	11.493		20.00
ATOM	4621	C1	SUG	1000	67.3		3.706	10.364		20.00
ATOM	4622	N	SUG	1000	67.8		2.445	9.937		20.00
ATOM	4623	C2	SUG	1000	66.4		4.224	9.501		20.00
ATOM	4624	C3	SUG	1000	65.8		5.499	9.765		20.00
ATOM	4625	C4	SUG	1000	66.2		6.212	10.884		20.00
MOTA	4626	C5	SUG	1000	67.2		5.690	11.736		20.00
ATOM	4627	C6	SUG	1000	66.1		3.220	8.401		20.00
ATOM	4628	0	SUG	1000	67.3		1.047	8.275		20.00
MOTA	4629	C7	SUG	1000	67.1		2.121	8.828		20.00
ATOM	4630	C8	SUG	1000	63.3		2.460	5.852		20.00
MOTA	4631	C9	SUG	1000	65.2		3.356	7.382		20.00

ATOM	4632	C10	SUG	1000	64.603	2.300	6.514	1.00 20.00
ATOM	4633	C11	SUG	1000	64.167	0.392	5.481	1.00 20.00
MOTA	4634	C12	SUG	1000	63.106	1.251	5.206	1.00 20.00
ATOM	4635	N13	SUG	1000	65.103	1.023	6.293	1.00 20.00
ATOM	4636	C14	SUG	1000	61.898	0.897	4.346	1.00 20.00
MOTA	4637	C15	SUG	1000	62.476	3.715	5.826	1.00 20.00
MOTA	4638	C16	SUG	1000	61.259	3.598	6.771	1.00 20.00
MOTA	4639	01	SUG	1000	60.814	5.963	6.429	1.00 20.00
ATOM	4640	C17	SUG	1000	60.520	4.912	6.988	1.00 20.00
ATOM	4641	02	SUG	1000	59.496	4.795	7.873	1.00 20.00
ATOM	4642	C	SUG	1001	5.413	2.967	18.087	1.00 20.00
MOTA	4643	Cl	SUG	1001	5.891	2.927	19.417	1.00 20.00
ATOM	4644	N	SUG	1001	5.553	2.021	20.431	1.00 20.00
ATOM	4645	C2	SUG	1001	6.828	3.875	19.872	1:00 20.00
ATOM	4646	C3	SUG	1001	7.304	4 884	18.988	1.00 20.00
MOTA	4647	C4	SUG	1001	6.822	4.909	17.678	1.00 20.00
MOTA	4648	C5	SUG	1001	5.890	3.964	17.233	1.00 20.00
MOTA	4649	C6	SUG	1001	7.145	3.576	21.318	1.00 20.00
ATOM	4650	0	SUG	1001	6.101	1.678	22.552	1.00 20.00
MOTA	4651	C7	SUG	1001	6.237	2.343	21.530	1.00 20.00
ATOM	4652	CB	SUG	1001	9.967	4.392	23.809	1.00 20.00
ATOM	4653	C9	SUG	1001	7.997	4.264	22.102	1.00 20.00
MOTA	4654	C10	SUG	1001	8.753	3.835	23.357	1.00 20.00
MOTA	4655	C11	SUG	1001	9.331	2.736	25.189	1.00 20.00
MOTA	4656	C).2		1001	10.320	3.689	24.962	1.00 20.00
MOTA	4657	N.T.3	•	1001	8.354	2.809	24.203	1.00 20.00
MOTA	4658	Cl4		1001	11.547	3.900	25.843	1.00 20.00
MOTA	4659	015		1001	10.759	5.550	23.175	1.00 20.00
ATOM	4660	C15	SUG	1001	11.987	5.063	22.373	1.00 20.00
ATOM	4661	O:L	SUG	1001	12.243	7.308	21.475	1.00 20.00
ATOM	4662	C1?	SUG	1001	12.621	6 142	21.504	1.00 20.00
ATOM	4663	02	SUG	1001	13.657	5.670	20.762	1.00 20.00

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TABLE 4

Atom		tom	A. A		x	Y	Z	occ	В	
No.		уре	Тур							
ATOM	1	N	GLU	1464	-13.576	17.066	8.598	1.00	57.39	
ATOM	2	CA	GLU	1464	-12.446	17.198	7.684	1.00	55.83	
MOTA	3	CB	GLU	1464	-11.381	18.127	8.275	1.00	56.73	
MOTA	4	С	GLU	1464	-11.845	15.833	7.341	1.00	55.07	
ATOM	5	0	GLU	1464	-11.722	15.504	6.165	1.00	59.74	
ATOM	6	N	LEU	1465	-11.518	15.023	8.347	1.00	50.12	
ATOM	. 7	CA	LEU	1465	-10.950	13.699	8.087	1.00	44.43	
ATOM	8	CB	LEU	1465	-10.155	13.196	9.291	1.00	43.28	
ATOM	9	CG	LEU	1465	-8.630	13.316	9.227	1.00	43.70	
ATOM	10	CD1	LEU	1465	-8.222	14.754	9.013	1.00	47.59	
ATOM	11	CD2	LEU	1465	-8.017	12.803	10.506	1.00	42.63	
MOTA	12	C	LEU	1465	-12.046	12.697	7.739	1.00	40.93	
ATOM	13	0	LEU	1465	-13.139	12.730	8.301	1.00	39.13	
ATOM	14	N	PRO	1466	-11.794	11.852	6.726		40.49	
ATOM	15	CD	PRO	1466	-10.612	11.884	5.844		39.07	
ATOM	16	CA	PRO	1466	-12.754	10.831	6.284		40.14	
ATOM	17	CB	PRO	1466	-12.152	10.331	4.981		40.90	
ATOM	18	CG	PRO	1466	-10.664	10.518	5.202		41.39	
ATOM	19	С	PRO	1466	-12.862	9.701	7.305		40.06	
ATOM	20	0	PRO	1466	-11.857	9 290	7.883		40.71	
ATOM	21	N	GLU	1467	-14.064	9.175	7.491		38.65	
ATOM	22	CA	GLU	1467	-14.255	8.126	8.467		39.24	
ATOM	23	СВ	GLU	1467	-15.722	8.054	8.873		45.06	
ATOM	24	CG	GLU	1467	-16.314	9.365	9.353		50.91	
ATOM	25	CD	GLU	1467	-17.789	9.252	9.699		53.51	
ATOM	26		GLU	1467	-18.379	8.170	9.504		54.15	
ATOM	27		GLU	1467	-18.369	10.250	10.160		53.10	
ATOM	28	C	GLU	1467	-13.808	6.777	7.914		36.09	
ATOM	29	0	GLU	1467	-13.922	6.529	6.711	1.00		
ATOM	30	N	ASP	1468	-13.272					
ATOM	31	CA	ASP	1468	-12.839	5.929	8.791	1.00		
ATOM	32	СВ	ASP	1468	-12.639	4.592	8.407	1.00		
ATOM	33	CG	ASP	1468	-11.328	4.515 3.207	8.186	1.00		
ATOM	34	OD1		1468			7.529	1.00		
ATOM	35	OD2		1468	-11.623	2.199	7.572	1.00		
ATOM	36	C C	ASP	1468	-9.777	3.187	6.962	1.00		
ATOM					-13.274	3.627	9.493	1.00		
	37	0	ASP	1468	-12.570	3.405	10.493	1.00		
ATOM	38	N	PRO	1469	-14.450	3.019	9.305	1.00		
ATOM	39	CD	PRO	1469	-15.396	3.175	8.183	1.00		
ATOM	40	CA	PRO	1469	-14.963	2.079	10.294	1.00	26.69	
ATOM	41	CB	PRO	1469	-16.255	1.586	9.641	1.00	28.81	
ATOM	42	CG	PRO	1469	-16.702	2.776	8.816	1.00	24.20	
ATOM	43	С	PRO	1469	-14.012	0.925	10.625	1.00	27.51	
ATOM	44	0	PRO	1469	-14.172	0.285	11.657	1.00	2 7 .60	
ATOM	45	N	ARG	1470	-13.075	0.642	9.720	1.00	26.49	
ATOM	46	CA	ARG	1470	-12.108	-0.435	9.935	1.00		

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MOTA 47 CB ARG 8.668 1.00 26.08 1470 -11.285 -0.691 MOTA 48 CG ARG 1470 -12.073 -1.125 7.439 1.00 30.77 MOTA 49 CD ARG 1470 -11.153 -1.257 6.213 1.00 31.66 MOTA 50 NE ARG 1470 -10.462 0.001 5.915 1.00 30.94 MOTA 51 CZ ARG 1470 -9.577 4.941 1.00 33.30 0.167 **MOTA** 52 NH1 ARG 1470 -9.249 -0.846 1.00 32.78 4.144 MOTA 53 NH2 ARG 1470 -8.990 1.346 4.779 1.00 27.16 MOTA 54 С ARG 1470 -11.116 -0.163 11.069 1.00 28.73 MOTA 55 ARG 0 1470 -10.588 -1.091 11.673 1.00 27.30 MOTA 56 N TRP 1471 -10.871 1.107 11.363 1.00 27.98 **ATOM** 57 CA TRP -9.892 1471 1.430 12.375 1.00 26.33 MOTA 58 CB TRP 1471 -8.642 1.964 11.671 1.00 23.87 MOTA -7.998 59 CG TRP -1471 --0.947 10.795 1.00 24.61 ATOM CD2 TRP 60 1471 -7.110 -0.104 11.205 1.00 23.32 **ATOM** 61 CE2 TRP 1471 -6.732 -0.807 10.041 1.00 24.34 MOTA 62 CE3 TRP 1471 -6.589 -0.509 12.438 1.00 21.39 MOTA 63 CD1 TRP 1471 -8.129 0.831 9.446 1.00 25.07 **ATOM** 64 NE1 TRP -7.369 1471 -6.220 8.980 1.00 26.82 **ATOM** 65 CZ2 TRP 1471 -5.860 -1.898 10.083 1 00 23.12 ATOM 66 CZ3 TRP 1471 -5.722 -1.589 12.473 1.00 21.02 ATOM CH2 TRP 67 1471 11.306 -5.364 -2.265 1.00 21.74 MOTA 68 C TRP 1471 -10.292 2.384 13.478 1.00 26.93 MOTA €9 o TRP 1471 -9.551 2.544 14.452 1.00 26.37 MOTA 70 N GLU 1472 -11.464 2.975 13.364 1.00 26.40 71 MOTA CA GLU 1472 -11.909 3.959 14.341 1.00 27.12 MOTA -13.168 72 CB GLU 1472 4.674 13.821 1.00 28.25 MOTA ?3 CG GLU 1472 -13.497 6.026 14.498 1.00 27.47 MOTA -12.611 74 CD GLU 1472 7.180 14.042 1.00 24.64 MOTA 75 OE1 GLU 1472 -11.877 7.039 13.042 1.00 24.60 MOTA 76 OE2 GLU 1472 -12.658 8.247 14.683 1.00 23.70 MOTA 77 С GLU 1472 -12.179 3.421 15.735 1.00 25.89 MOTA 78 0 GLU 1472 -12.795 2.373 15.891 1.00 27.74 ATOM. 79 N LEU 1473 -11.689 4.121 16.745 1.00 25.95 **ATOM** 80 CA LEU 1473 -11.961 3.740 18.129 1.00 27.45 MOTA 81 СВ LEU 1473 -10.707 3.311 18.890 1.00 24.99 MOTA 82 CG LEU 1473 -10.958 3.090 20.392 1.00 21.80 **ATOM** 83 CD1 LEU 1473 -11.551 1.696 20.627 1.00 20.63 MOTA 84 CD2 LEU 1473 -9.646 3.199 21.157 1.00 22.34 **ATOM** 85 C LEU 5.008 18.752 1473 -12.478 1.00 29.33 MOTA 86 0 LEU 1473 -12.007 6.101 18.405 1.00 27.56 **ATOM** 87 N PRO 1474 -13.529 4.896 19.585 1.00 30.07 **ATOM** 88 CD PRO 1474 -14.380 3.704 19.737 1.00 29.18 **ATOM** 89 CA PRO 1474 -14.124 6.051 20.267 1.00 29.03 **ATOM** 90 CB PRO 1474 -15.266 5.406 21.062 1.00 26.83 MOTA CG PRO 91 1474 -15.701 4.307 20.158 1.00 26.35 MOTA С 92 PRO 1474 -13.099 6.715 21.178 1.00 31.01 **ATOM** 93 0 PRO 6.042 21.850 1474 -12.310 1.00 33,14 MOTA 94 N ARG 1475 8.038 -13.110 21.178 1.00 31.33 **ATOM** 95 CA ARG 1475 -12.181 8.810 21.973 1.00 32.99 MOTA 96 CB ARG 1475 21.791 -12.442 10.292 1.00 35.87 MOTA 97 CG ARG 1475 -12.082 10.729 20.413 1.00 43.88 MOTA 98 CD ARG 1475 -11.984 12.228 20.247 1.00 44.84

ATOM	99	NE	ARG	1475	-11.665	12.499	18.846	1.00 48.59
ATOM	100	CZ	ARG	1475	-10.435	12.663	18.374	1.00 46.00
ATOM	101	NHI	ARG	1475	-9.400	12.618	19.202	1.00 46.56
ATOM	102	NH2	ARG	1475	-10.241	12.746	17.065	1.00 44.18
ATOM	103	C	ARG	1475	-12.175	8.456	23.442	1.00 35.47
ATOM	104	0	ARG	1475	-11.115	8.400	24.072	1.00 37.44
ATOM	105	N	ASP	1476	-13.347	8.134	23.974	1.00 35.04
ATOM	106	CA	ASP	1476	-13.468	7.800	25.380	1.00 34.30
ATOM	107	CB	ASP	1476	-14.940	7.853	25.797	1.00 36.89
ATOM	108	CG	ASP	1476	-15.796	6.818	25.089	1.00 38.67
ATOM	109	OD1	ASP	1476	-15.288	6.056	24.234	1.00 41.19
ATOM	110	OD2	ASP	1476	-16.995	6.758	25.406	1.00 48.08
ATOM	111	С	ASP	1476	-12.858	6.457	25.770	1.00 33.67
ATOM	112	O	ASP	1476	-12.830	6.109	26.949	1.00 36.57
ATOM	113	N	ARG	1477	-12.441	5.670	24.781	1.00 32.72
ATOM	114	CA	ARG	1477	-11.828	4.370	25.033	1.00 29.68
ATOM	115	CB	ARG	1477	-12.117	3.418	23.886	1.00 25.53
ATOM	116	CG	ARG	1477	-13.564	3.189	23.599	1.00 23.83
ATOM	117	CD	ARG	1477	-14.234	2.525	24.772	1.00 26.80
MOTA	118	NE	ARG	1477	-14.493	3.485	25.842	1.00 27.24
MOTA	119	CZ	ARG	1477	-14.818	3.145	27.085	1.00 27.41
ATOM	120	NH1	ARG	1477	-14.931	1.874	27.438	1.00 29.00
ATOM	121		ARG	1477	-15.005	4.095	27.985	1.00 25.85
ATOM	122	C	ARG	1477	-10.316	4.489	25.177	1.00 30.44
ATOM	123	0	ARG	1477	-9.616	3.515	25.461	1.00 32.78
ATOM	124	N	LEU	1478	-9.800	5.690	25.002	1.00 30.39
ATOM	125	CA	LEU	1478	- 8.370	5.883	25.080	1 00 31.96
ATOM	126	CB	LEU	1478	-7.886	6.508	23.771	1.00 30.43
ATOM	127	CG	LEU	1478	-6.400	6.424	23.431	1.00 31.90
MOTA	128		LEU	1478	-5.939	4.964	23.382	1.00 28.92
ATOM	129		LEU	1478	-6.159	7.115	22.102	1.00 33.55
ATOM	130	C	LEU	1478	-7.974	6.757	26.265	1.00 33.60
ATOM	131	0	LEU	1478	-8.193	7.972	26.251	1.00 33.96
ATOM	132	N	VAL	1479	-7.416	6.140	27.305	1.00 33.54
ATOM	133	CA	VAL	1479	-6.974	6.902	28.468	1.00 32.52
ATOM	134	CB	VAL	1479	-7.085	6.089	29.757	1.00 32.76
ATOM	135		VAL	1479	-6.728	6.973	30.926	1.00 33.27
ATOM	136		VAL	1479	-8.493	5.537	29.913	1.00 30.15
ATOM	137	C	VAL	1479	-5.529	7.341	28.239	1.00 34.24
ATOM	138	0	VAL	1479	-4.581	6.546	28.350	1.00 32.24
ATOM	139	N	LEU	1480	-5.381	8.607	27.867	1.00 35.88
ATOM ATOM	140	CA	LEU	1480	-4.077	9.192	27.569	1.00 38.43
	141	CB	LEU	1480	-4.241	10.541	26.855	1.00 36.93
ATOM	142	CG	LEU	1480	-4.828	10.535	25.435	1.00 35.67
ATOM	143		LEU	1480	-4.762	11.952	24.907	1.00 32.47
ATOM ATOM	144		LEU	1480	-4.037	9.613	24.499	1.00 33.60
	145	C	LEU	1480	-3.144	9.324	28.768	1.00 39.70
ATOM	146	O N	LEU	1480	-3.511	9.912	29.784	1.00 39.88
ATOM	147	N	GLY	1481	-1.912	8.842	28.610	1.00 39.70
ATOM	148	CA	GLY	1481	-0.960	8.896	29.700	1.00 41.31
ATOM	149	C	GLY	1481	0.349	9.633	29.474	1.00 44.39
ATOM	150	0	GLY	1481	0.429	10.626	28.744	1.00 45.69

ATOM	151	N	LYS	1482	1.389	9.122	30.124	1.00	44.73
ATOM	152	CA	LYS	1482	2.728	9.700	30.069	1.00	46.91
ATOM	153	CB	LYS	1482	3.649	8.934	31.023	1.00	51.20
MOTA	154	CG	LYS	1482	5.135	9.056	30.744	1.00	57.10
ATOM	155	CD	LYS	1482	5.878	7.826	31.248	1.00	60.81
ATOM	156	CE	LYS	1482	5.430	6.567	30.515	1.00	61.24
MOTA	157	NZ	LYS	1482	6.235	5.375	30.912	1.00	65.39
MOTA	158	C	LYS	1482	3.370	9.782	28.681		46.09
ATOM	159	0	LYS	1482	3.440	8.782	27.944		42.98
ATOM	160	N	PRO	1483	3.886	10.969	28.324	1.00	46.65
ATOM	161	CD	PRO	1483	3.910	12.184	29.152	1.00	46.11
MOTA	162	CA	PRO	1483	4.536	11.212	27.036		45.96
ATOM	163	СВ	PRO	1483	5.015	12.660	27.172		43.59
ATOM	164	CG	PRO	1483	4.041	13.253	28.122	1.00	45.37
MOTA	165	C	PRO	1483	5.739	10.279	26.912		46.43
MOTA	166	0	PRO	1483	6.506	10.139	27.861		44.77
MOTA	167	N	LEU	1484	5.844	9.579	25.786		48.21
MOTA	168	CA	LEU	1484	6.978	8.684	25.554	1.00	
MOTA	169	CB	LEU	1484	6.543	7.426	24 811	1.00	49.38
ATOM	170	CG	LEU	1484	5.655	6.437	25.576		50.15
ATOM	171	CD1	LEU	1484	5.067	5.422	24.615		44.90
ATOM	172	CD2	LEU	1484	5.446	5.750	26.669		44.60
ATOM	173	С	LEU	1484	.8.058	9.419	24.764	1.00	53.33
ATOM	174	0	LEU	1484	9.241	9.116	24.896	1.00	51.94
MOTA	175	Ŋ	GLY	1485	7.643	10.376	23.931	1.00	57.68
MOTA	176	CA	GLY	1485	8.603	11.140	23.149	1.00	60.27
MOTA	177	С	GLY	1485	7.997	11.946	22.016	1.00	62.66
ATOM	178	0	GLY	1485	6.774	12.090	21.924	1.00	64.91
MOTA	179	N	GLN	1491	4.704	14.425	13.904	1.00	47.86
MOTA	180	CA	GLN	1491	4.339	13.869	20.206	1.00	44.42
MOTA	181	CB	GLN	1491	3.373	14.829	20.918	1.00	44.31
ATOM	182	С	GLN	1491	3.755	12.433	20.170	1.00	43.09
MOTA	183	0	GLN	1491	2.807	12.150	19.426	1.00	43.67
MOTA	184	N	VAL	1492	4.338	11.542	20.974	1.00	40.40
ATOM	185	CA	VAL	1492	3.903	10.143	21.101	1.00	39.95
ATOM	186	CB	VAL	1492	4.962	9.119	20.673	1.00	37.64
MOTA	187	CG1	VAL	1492	4.416	7.721	20.897	1.00	34.94
ATOM	188	CG2	VAL	1492	5.336	9.296	19.233	1.00	40.26
ATOM	189	С	VAL	1492	3.720	9.905	22.586	1.00	40.23
MOTA	190	0	VAL	1492	4.679	10.038	23.355	1.00	40.41
MOTA	191	N	VAL	1493	2.516	9.518	22.993	1.00	38.15
ATOM	192	CA	VAL	1493	2.250	9.291	24.405	1.00	37.11
MOTA	193	CB	VAL	1493	1.131	10.245	24.924	1.00	37.83
MOTA	194		VAL	1493	1.386	11.656	24.422	1.00	36.45
ATOM	195	CG2	VAL	1493 -	0.252	9.769	24.508	1.00	39.28
ATOM	196	С	VAL	1493	1.854	7.844	24.701	1.00	36.02
ATOM	197	0	VAL	1493	1.450	7.118	23.797	1.00	37.17
ATOM	198	N	LEU	1494	2.052	7.418	25.944	1.00	32. 7 7
ATOM	199	CA	LEU	1494	1.645	6.081	26.335	1.00	30.87
MOTA	200	СВ	LEU	1494	2.445	5.587	27.550		27.22
ATOM	201	CG	LEU	1494	1.970	4.250	28.141	1.00	28.67
ATOM	202	CD1	LEU	1494	2.124	3.132	27.129	1.00	27.40

ATOM	203	CD2	LEU	1494	2.736	3.904	29.377	1.00 28.84
ATOM	204	C	LEU	1494	0.173	6.256	26.701	1.00 31.18
ATOM	205	0	LEU	1494	-0.249	7.344	27.119	1.00 30.88
MOTA	206	N	ALA	1495	-0 626	5.223	26.477	1.00 30.40
ATOM	207	CA	ALA	1495	-2.044	5.307	26.817	1.00 28.30
ATOM	208	CB	ALA	1495	-2.815	5.999	25.691	1.00 27.35
MOTA	209	С	ALA	1495	-2.608	3.919	27.057	1.00 26.32
MOTA	210	0	ALA	1495	-1.926	2.915	26.846	1.00 24.54
ATOM	211	N	GLU	1496	-3.836	3.867	27.552	1.00 28.11
MOTA	212	CA	GLU	1496	-4.514	2.603	27.793	1.00 29.22
MOTA	21.3	CB	GLU	1496	-4.841	2.441	29.272	1.00 31.77
ATOM	214	CG	GLU	1496	-3.627	2.233	30.140	1.00 37.26
MOTA	215	CD	GLU	1496	-3.950	2.405	.31.613	1.00 39.77
ATOM	216	OE1	GLU	1496	-4.322	3.534	31.999	1.00 37.54
MOTA	217	OE2		1496	-3.835	1.417	32.378	1.00 41.52
MOTA	218	С	GLU	1496	-5.799	2.594	26.970	1.00 29 76
ATOM	219	O	GLU	1496	-6.593	3.543	27.020	1.00 31.39
MOTA	220	N	ALA	1497	-5.961	1.561	26.153	1.00 29.55
ATOM	221	CA	ALA	1497	-7.139	1.426	25.324	1.00 28.69
ATOM	222	CB	ALA	1497	-6.742	0.969	23.930	1.00 23.86
ATOM	223	C	ALA	1497	-8.068	J.418	25.965	1.00 29.51
ATOM	224	O	ALA	1497	-7.657	-0.762	26.278	1.00 30.40
ATOM	225	N	ILE	1498	-9.313	0.823	26.201	1.00 31.33
ATOM	226	CA	lLE	1498	-10.302	-0.064	26.811	1.00 32.30
ATOM	227	CB	ILE	1498	-11.359	0.727	27.619	1.00 33.61
ATOM	228	CG2		1498	-12.233	-0.246	28.439	1.00 34.55
ATOM	229	CG1		1498	-10.690	1.745	28.545	1.00 31.99
MOTA	230	CD1		1498	-11.663	2.730	29.155	1.00 26.68
ATOM	231	C	ILE	1498	-11.023	-0.777	25.673	1.00 32.69
ATOM	232	0	ILE	1498	-11 644	-0.134	24.838	1.00 32.03
ATOM ATOM	233	N	GLY	1499	-10.917	-2.095	25.610	1.00 37.34
ATOM	234 235	CA C	GLY	1499	-11.588	-2.822	24.554	1.00 44.45
ATOM	236	0	GLY	1499	-10.709	-3.193	23.372	1.00 50.75
ATOM	237	N	GLY LEU	1499	-9.993	-4.205	23.438	1.00 53.68
ATOM	238	CA		1500 1500	-10.729	-2.370	22.321	1.00 51.14
ATOM	239	CB	LEU LEU		-9.963	-2.613	21.087	1.00 51.15
ATOM	240	CG	LEU	1500 1500	-8.445 -7.516	-2.677	21.345	1.00 50.85
ATOM	241		LEU	1500	~7.516	-1.463	21.166	1.00 49.05
ATOM	242		LEU	1500	-6.082 -7.703	-1.946 -0.783	21.263	1.00 44.92
ATOM	243	c	LEU	1500	-10.420	-3.891	19.824 20.376	1.00 44.03
ATOM	244	o	LEU	1500	-10.544	-4.966	20.376	1.00 50.50
ATOM	245	N	PRO	1505	-13.321	-5.777	25.373	1.00 49.92 1.00 48.57
ATOM	246	CD	PRO	1505	-13.937	-7.111	25.286	
ATOM	247	CA	PRO	1505	-14.289			1.00 50.09
ATOM	248	СВ	PRO	1505	-15.630	-4.776 -5.503	25.848 25.710	1.00 46.31 1.00 45.25
ATOM	249	CG	PRO	1505	-15.271	-6.918		
ATOM	250	C	PRO	1505	-14.010	-4.321	26.025 27.294	1.00 48.85 1.00 43.31
ATOM	251	0	PRO	1505	-14.010	-3.122	27.294	1.00 43.31
ATOM	252	N	ASN	1506	-13.712	-5.272	28.178	1.00 42.84
ATOM	253	CA	ASN	1506	-13.712	-4.945	29.571	1.00 40.46
ATOM	254	CB	ASN	1506	-14.302	-5.776		
			.1011	100	- 14.302	-3.776	30.512	1.00 43.55

ATOM	255	CG	ASN	1506	-15.760	-5.436	30.382	1.00 42.68
ATOM	256	OD1	ASN	1506	-16.141	-4.269	30.316	1.00 47.11
MOTA	257	ND2	ASN	1506	-16.591	-6.461	30.323	1.00 45.66
MOTA	258	С	ASN	1506	-11.962	-5.097	29.957	1.00 42.89
ATOM	259	0	ASN	1506	-11.617	-5.221	31.137	1.00 43.23
MOTA	260	N	ARG	1507	-11.099	-5.066	28.949	1.00 42.72
MOTA	261	CA	ARG	1507	-9.661	-5.186	29.145	1.00 42.24
ATOM	262	CB	ARG	1507	-9.144	-6.384	28.353	1.00 50.39
ATOM	263	CG	ARG	1507	-9.407	-7.728	28.992	1.00 60.88
ATOM	264	CD	ARG	1507	-8.357	-8.063	30.038	1.00 67.47
MOTA	265	NE	ARG	1507 .	-8.566	-9.401	30.574	1.00 74.19
MOTA	266	CZ	ARG	1507	-8.012	-9.861	31.691	1.00 79.97
ATOM	267	NH1	ARG	1507	.7.193	-9.093	32:406	1.00-81.67
ATOM	268	NH2	ARG	1507	-8.338	~ 3.1 . 068	32.134	1.00 82.38
ATOM	269	С	ARG	1507	-8.982	-3.940	28.611	1.00 38.15
ATOM	270	0	ARG	1507	-9.458	-3.354	27.642	1.00 36.46
ATOM	271	N	VAL	1508	·7.927	-3.491	29.279	1.00 35.19
ATOM	272	CA	VAL	1508	-7190	-2.335	28.782	1.00 33.82
ATOM	273	CB	VAL	1508	-6.824	-1.296	29.883	1.00 30.19
ATOM	274	CG1	VAL	1508	-8.072	-0.723	30.498	1.00 34.68
ATOM	275	CG2	VAL	1.508	-5.948	-1.900	30.938	1.00 28.53
ATOM	276	C	VAL	1508	5.912	-2.869	28.155	1.00 33.91
ATOM	277	0	VAL	1508	-5.392	-3 926	28.555	1.60 34.02
ATOM	278	N	THR	1509	-5.427	-2.152	27.154	1.00 31.32
ATOM	279	CA	THR	1509	-4.206	-2.527	26.476	1.00 30.47
MOTA	280	CB	THR	1509	-4.492	-3.015	25.031	1.00 30.88
ATOM	381	OG1	THR	1509	-5.522	-4.008	25.066	1.00 33.90
ATOM	282	CG2	THR	1509	~3.255	-3.648	24.411	1.00 24.49
MOTA	283	С	THR	1509	-3.323	-1.300	26.419	1.00 28.74
ATOM	284	0	THR	1509	-3,774	-0.219	26.039	1.00 27.29
ATOM	285	N	LYS	1510	-2.092	-1.432	26.893	1.00 27.23
MOTA	286	CA	LYS	1510	-1.162	-0.325	26.831	1.00 30.55
ATOM	287	СВ	LYS	1510	0.092	-0.595	27.648	1.00 27.23
MOTA	288	CG	LYS	1510	-0.117	-0.460	29.135	1.00 34.33
ATOM	289	CD	LYS	1510	1.191	-0.614	29.896	1.00 40.49
ATOM	290	CE	LYS	1510	1.065	-1.603	31.062	1.00 48.28
ATOM	291	NZ	LYS	1510	0.318	-1.067	32.245	1.00 51.03
MOTA	292	С	LYS	1510	-0.813	-0.213	25.355	1.00 29.64
MOTA	293	0	LYS	1510	0.521	-1.218	24.700	1.00 28.00
MOTA	294	N	VAL	1511	-0.904	1.004	24.836	1.00 30.10
ATOM	295	CA	VAL	1511	-0.625	1.305	23.446	1.00 30.13
MOTA	296	СВ	VAL	1511	-1.951	1.464	22.636	1.00 30.13
ATOM	297		VAL	1511	-2.719	0.143	22.615	1.00 30.42
ATOM	298		VAL	1511	-2.829	2.629	23.223	1.00 30.42
ATOM	299	C	VAL	1511	0.150	2.626	23.365	
ATOM	300	0	VAL	1511	0.130	3.346	24.360	1.00 30.51
ATOM	301	N	ALA	1512	0.679	2.935		1.00 31.09
ATOM	302	CA	ALA	1512	1.408		22.185	1.00 28.30
ATOM	303	CB	ALA			4.173	21.979	1.00 25.23
				1512	2.740	3.889	21.331	1.00 23.82
ATOM	304	C	ALA	1512	0.535	5.012	21.057	1.00 25.50
ATOM	305	0	ALA	1512	0.033	4.515	20.061	1.00 27.06
MOTA	306	N	VAL	1513	0.351	6.281	21.404	1.00 29.37

MOTA 307 CA VAL 1513 -0.477 7.199 20.625 1.00 31.53 MOTA 308 CB VAL 1513 -1.588 21.504 1.00 32.26 7.843 MOTA 309 CG1 VAL 1513 -2.453 8.775 20.684 1.00 34.37 **ATOM** 310 CG2 VAL 1513 -2.452 6.776 22.152 1.00 33.42 MOTA С VAL 1513 0.347 311 8.328 20.006 1.00 33.34 MOTA 312 0 VAL 1513 1.030 9.064 20.719 1.00 32.35 **MOTA** 1514 313 N LYS 0.321 8.423 18.680 1.00 36.65 MOTA CA LYS 1514 314 1.022 9.466 17.929 1.00 37.26 MOTA 315 CB LYS 1514 1.541 8.917 16.606 1.00 36.21 MOTA CG LYS 1514 1.00 39.32 316 2.524 7.792 16.800 MOTA 317 CD LYS 1514 2.725 6.998 15.535 1.00 42.59 MOTA 318 CE LYS 1514 3.245 7.860 14.416 1.00 44.71 MOTA NZ - LYS 319 1514------- 4.408 8.680 14.844 1.00 38.78 ATOM 320 C LYS 1514 0.020 10.574 17.653 1.00 37.21 MOTA 321 0 LYS 1514 -1.095 10.305 17.192 1.00 37.39 MOTA 322 N MET 1515 0.433 11.812 17.908 1.00 39.05 MOTA 323 CA MET 1515 -0.419 12.981 17.713 1.00 41.68 ATOM 324 CB MET 1515 -1.162 13.299 18.991 1.00 41.07 **ATOM** 325 CG MET 1515 -0.251 13.641 20.139 1.00 40.69 ATOM SD 1515 326 MET -1.271 13.763 21.571 1.00 41.18 MOTA 327 CE 1515 MET -1.523 12.018 21.959 1.00 40.98 MOTA С 328 MET 1515 0.397 14.197 17.321 1.00 44.66 MOTA 329 0 1515 1.606 MET 14.255 17.550 1.00 43.83 MOTA 330 N LEU 1516 -0.288 15.182 16.747 1.00 50.63 ATOM 331 CA LEU 1516 0.349 16.423 16.312 1.00 52.21 MOTA 332 CB LEU 1516 ..0.513 17.129 15.255 1.00 50.18 MOTA 333 CG LEU 1516 -0.757 16.463 13.904 1.00 50.25 MOTA 334 CD1 LEU 1516 -1.733 17.298 13.114 1.00 51.02 **ATOM** 335 CD2 LEU 1516 0.555 16.329 13.163 1.00 51.60 MOTA 336 C LEU 1516 0.549 17.391 17.473 1.00 54.25 **ATOM** 337 LEU 0 1516 -0.143 17.326 19.488 1.00 52.52 MOTA 338 N LYS 1517 1.500 18.299 17.302 1.00 59.09 MOTA 339 CA LYS 1517 1.773 19.315 18.313 1.00 62.57 MOTA 340 CB LYS 1517 3.220 19.813 18.222 1.00 66.29 MOTA 341 CG LYS 1517 4.281 18.810 18.663 1.00 70.96 MOTA 342 CD LYS 1517 5.666 19.197 18.130 1.00 74.61 MOTA 343 CE LYS 1517 6.711 18.118 18.414 1.00 78.21 MOTA 344 NZ LYS 1517 8.020 18.410 17.751 1.00 77.95 345 MOTA C LYS 1517 0.824 20.474 18.037 1.00 63.07 346 MOTA 0 LYS 1517 0.226 20.557 16.960 1.00 63.68 MOTA 347 N SER 1518 0.720 21.391 18.987 1.00 64.54 MOTA 348 CA SER 1518 -0.167 22.543 18.848 1.00 67.29 MOTA 349 CB SER 1518 -0.085 23.439 20.090 1.00 65.14 MOTA 350 С SER 1518 0.124 23.382 17.609 1.00 69.48 ATOM 351 0 SER 1518 -0.798 23.843 16.938 1.00 71.85 MOTA 352 N. ASP 1519 1.402 23.530 17.280 1.00 70.88 MOTA 353 CA ASP 1519 1.802 24.326 16.127 1.00 72.00 **ATOM** 354 CB ASP 1519 3.162 24.973 16.385 1.00 72.61 MOTA 355 C **ASP** 1519 1.861 23.548 14.817 1.00 72.32 **ATOM** 356 0 ASP 1519 2.432 24.035 13.844 1.00 73.72 MOTA 357 N ALA 1520 1.322 22.332 14.798 1.00 72.11 **ATOM** 358 CA ALA 1520 1.344 21.508 13.595 1.00 71.13

ومراعات والمملف السراوات المنافي المنافي

ATOM	359	СВ	ALA	1520	0.659	20.173	13.855	1.00 71.01
ATOM	360	С	ALA	1520	0.666	22.242	12.440	1.00 69.96
ATOM	361	0	ALA	1520	-0.314	22.962	12.639	1.00 71.41
ATOM	362	N	THR	1521	1.230	22.101	11.249	1.00 67.39
ATOM	363	CA	THR	1521	0.676	22.726	10.064	1.00 66.23
ATOM	364	CB	THR	1521	1.798	23.167	9.132	1.00 66.40
ATOM	365	OG1	THR	1521	2.521	22.016	9.680	1.00 70.07
ATOM	366	CG2	THR	1521	2.741	24.070	9.867	1.00 66.67
ATOM	367	С	THR	1521	-0.150	21.665	9.364	1.00 65.62
ATOM	368	0	THR	1521	-0.093	20.493	9.740	1.00 66.78
ATOM	369	N	GLU	1522	-0.893	22.057	8.330	1.00 63.60
ATOM .	370	CA	GLU	1522	-1.698	21.095	7.584	1.00 62.25
ATOM	.371	CB	GLU	1522	-2.560	21.802	6.531	1.00 64.02
ATOM	372	C	GLU	1522	-0.768	20.051	6.942	1.00 60.41
ATOM	373	0	GLU	1522	-1.161	18.906	6.738	1.00 61.94
ATOM	374	N	LYS	1523	0.475	20.441	6.662	1.00 56.47
MOTA	375	CA	LYS	1523	1.449	19.529	6.080	1.00 54.53
ATOM	376	CB	LYS	1523	2.739	20.273	5.713	1.00 57.44
ATOM	377	CG	LYS	1523	3.897	19.381	5 219	1.00 61.49
ATOM	378	CD	LYS	1523	3.482	18.451	4.071	1.00 64.66
ATOM	379	CE	LYS	1523	4.681	17.723	3.469	1.00 68.18
ATOM	380	NZ	LYS	1523	4.252	16.704	2.458	1.00 73.23
ATOM	381	С	LYS	1523	1.72B	18.474	7.135	1.00 52.30
ATOM	382	0	LYS	1523	1.757	17.280	6.832	1.00 54.59
ATOM	383	N	ASP	1524	1.899	18.921	8.376	1.00 47.78
ATOM	384	CA	ASP	1524	2.147	18.023	9.493	1.00 45.55
ATOM	385	CB	ASP	1524	2.380	18.815	10.783	1.00 47.64
ATOM	386	CG	ASP	1524	3.744	19.511	10.817	1.00 49.50
ATOM	387	OD1	ASP	1524	3.849	20.580	11.460	1.00 47.22
ATOM	388	OD2	ASP	1524	4.715	18.984	10.230	1.00 52.84
ATOM	389	С	ASP	1524	0.968	17.054	9.661	1.00 43.55
ATOM	390	0	ASP	1524	1.157	15.890	10.007	1.00 43.98
ATOM	391	N	LEU	1525	-0.240	17.541	9.391.	1.00 40.77
ATOM	392	CA	LEU	1525	-1.438	16.713	9.483	1.00 40.28
MOTA	393	CB	LEU	1525	-2.701	17.592	9.411	1.00 40.54
ATOM	394	CG	LEU	1525	-4.100	16.957	9.403	1.00 40.33
MOTA	395	CD1		1525	-4.289	15.933	10.514	1.00 42.75
ATOM	396		LEU	1525	-5.120	18.044	9.524	1.00 36.98
MOTA	397	С	LEU	1525	-1.417	15.699	8.343	1.00 40.19
ATOM	398	0	LEU	1525	-1.682	14.525	8.557	1.00 41.90
ATOM	399	N	SER	1526	-1.064	16.158	7.147	1.00 42.13
ATOM	400	CA	SER	1526	-1.002	15.315	5.954	1.00 44.75
MOTA	401	CB	SER	1526	-0.582	16.136	4.723	1.00 49.61
MOTA	402	OG	SER	1526	-1.538	17.100	4.352	1.00 59.95
ATOM	403	С	SER	1526	-0.007	14.193	6.144	1.00 42.71
ATOM	404	O .	SER	1526	-0.297	13.047	5.840	1.00 45.33
ATOM	405	N	ASP	1527	1.167	14.527	6.655	1.00 40.97
ATOM	406	CA	ASP	1527	2.210	13.546	6.867	1.00 41.03
ATOM	407		ASP	1527	3.497	14.235	7.316	1.00 45.30
MOTA	408	CG	ASP	1527	4.083	15.147	6.235	1.00 47.84
ATOM	409	OD1		1527	3.700	15.041	5.047	1.00 48.84
MOTA	410	OD2	ASP	1527	4.957	15.966	6.600	1.00 49.11

ATOM	411	C	ASP	1527	1.782	12.485	7.858	1.00 39.01
ATOM	412	0	ASP	1527	2.021	11.298	7.651	1.00 40.04
MOTA	413	N	LEU	1528	1.094	12.917	8.909	1.00 35.93
MOTA	414	CA	LEU	1528	0.594	12.004	9.927	1.00 36.48
ATOM	415	CB	LEU	1528	-0.008	12.784	11.107	1.00 36.51
ATOM	416	CG	LEU	1528	-0.436	11.961	12.326	1.00 40.56
ATOM	417	CD1	LEU	1528	0.650	10.955	12.692	1.00 42.00
MOTA	418	CD2	LEU	1528	-0.770	12.877	13.499	1.00 38.25
ATOM	419	C	LEU	1528	-0.453	11.065	9.309	1.00 35.25
ATOM	420	0	LEU	1528	-0.442	9.855	9.566	1.00 36.37
ATOM	421	N	ILE	1529	-1.311	11.614	8.453	1.00 33.10
MOTA	422	CA	ILE	1529	-2.365	10.839	7.805	1.00 32.32
ATOM	423	CB	ILE	1529	-3.364	11.732	7.012	1.00 31.17
ATOM	424	CG2	ILE	1529	-4.311	10.861	6.187	1.00 32.01
ATOM	425	CG1	ILE	1529	-4.193	12.579	7.983	1.00 31.35
ATOM	426	CD1	ILE	1529	-5.024	13.662	7.335	1.00 32.59
ATOM	427	C	ILE	1529	-1.732	9.825	6.877	1.00 33.44
ATOM	428	0	ILE	1529	-2.148	8:667	ő.860	1.00 35.41
ATOM	429	N	SER	1530	-0.733	10.269	6.108	1.00 33.40
ATOM	430	ÇA	SER	1530	0.007	9.414	5.171	1.00 34.34
MOTA	431	CB	SER	1530	1.126	10.197	4.495	1.00 38.37
ATOM	432	OG	SER	1530	0.605	11.332	3.835	1.00 46.02
ATOM	433	C	SER	1530	0.614	8.208	5.968	1.00 30.41
MOTA	434	0	SER	1530	0.494	7.083	5.376	1.00 30.50
ATOM	435	N	GLU	1531	1.256	8.449	7.010	1.00 27.40
ATOM	436	CA	GLU	1531	1.865	7.369	7.766	1.00 28.90
ATOM	437	CB	GLU	1531	2.629	7.907	8.973	1.00 28.45
ATOM	438	CG	GLU	1531	3.263	6.812	9.825	1.00 29.33
ATOM	439	CD	GLU	1531	4.094	7.344	10.979	1.00 31.14
ATOM	440	OE1	GLU	1531	4.913	6.561	11.495	1.06 33.14
MOTA	441	OE2	GLU	1531	3.940	8.522	11.378	1.00 31.11
MOTA	442	C	GLU	1531	0.824	6.351	8.215	1.00 30.88
ATOM	443	0	GLU	1531	1.118	5.146	8.259	1.00 32.35
MOTA	444	N	MET	1532	-0.377	6.832	8.553	1.00 29.86
ATOM	445	CA	MET	1532	-1.476	5.966	8.996	1.00 30.01
MOTA	446	CB	MET	1532	-2.608	6.800	9.596	1.00 29.58
ATOM	447	CG	MET	1532	-3.761	5.968	10.146	1.00 31.20
ATOM	448	SD	MET	1532	-5.095	6.973	10.779	1.00 29.37
ATOM	449	CE	MET	1532	-5.271	8.228	9.489	1.00 21.59
ATOM	450	С	MET	1532	-2.002	5.145	7.814	1.00 29.60
MOTA	451	0	MET	1532	-2.131	3.923	7.893	1.00 29.68
ATOM	452	N	GLU	1533	-2.257	5.824	6.702	1.00 30.38
MOTA	453	CA	GLU	1533	-2.755	5.176	5.495	1.00 30.12
ATOM	454	CB	GLU	1533	-2.987	6.221	4.423	1.00 25.79
MOTA	455	CG	GLU	1533	-4.117	7.154	4.784	1.00 26.67
ATOM	456	CD	GLU	1533	-5.420	6.405	5.064	1.00 29.90
ATOM	457	OE1		1533	-5.923	5.696	4.166	1.00 29.93
ATOM	458	OE2		1533	-5.939	6.518	6.197	1.00 29.10
MOTA	459	С	GLU	1533	-1.787	4.120	5.003	1.00 30.32
MOTA	460	0	GLU	1533	-2.197	3.043	4.563	1.00 32.06
MOTA	461	N	MET	1534	-0.500	4.435	5.136	1.00 29.97
ATOM	462	CA	MET	1534	0.606	3.571	4.737	1.00 31.22

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ATOM	463	СВ	MET	1534	1.918	4.305	4.985	1.00	33.86
ATOM	464	CG	MET	1534	3.118	3.487	4.675	1.00	40.40
ATOM	465	SD	MET	1534	3.528	3.627	2.982	1.00	48.27
ATOM	466	CE	MET	1534	5.215	4.257	3.155	1.00	42.49
ATOM	467	С	MET	1534	0.565	2.304	5.581	1.00	30.90
ATOM	468	0	MET	1534	0.596	1.193	5.050	1.00	33.24
MOTA	469	N	MET	1535	0.493	2.485	6.896	1.00	29.07
ATOM	470	CA	MET	1535	0.417	1.354	7.813	1.00	28.82
MOTA	471	CB	MET	1535	0.325	1.829	9.274	1.00	28.87
ATOM	472	CG	MET	1535	1.622	2.434	9.803	1.00	28.16
ATOM	473	SD	MET	1535	1.674	2.633	11.595	1.00	30.96
ATOM	474	CE	MET	1535	1.393	4.335	11.729	1.00	27.69
ATOM	475	C	MET	1535	-0.777	0.460	7.445	1.00	28.59
ATOM	476	0	MET	1535	-0.682	- 0.774	7.530	1.00	30.37
MOTA	477	N	LYS	1536	-1.885	1.072	7.019	1.00	26.53
MOTA	478	CA	LYS	1536	-3.078	0.315	6.608		27.60
MOTA	479	CB	LYS	1536	-4.237	1.253	6.283	1.00	25.88
ATOM	480	CG	LYS	1536	-4.807	1.947	7.479	1.00	23.80
MOTA	481	CD	LYS	1536	-5.925	2.857	7.061	3001	21.64
ATOM	482	CE	LYS	1536	-6.402	3.674	8.225	1.00	21.83
MOTA	483	NZ	LYS	1536	-7.469	4.594	7.796	1.00	26.27
MOTA	484	C	LYS	1536	-2.813	-0.573	5.397	1.00	27.49
ATOM	485	၁	LYS	1536	-3.150	-1.756	5 393	1.00	29.24
ATOM	486	N	MET	1537	-2.186	-0.014	4.372	1.00	27.89
ATOM	487	CA	MET	1537	-1.890	0.783	3.172	1.00	29.12
MOTA	488	CB	MET	1537	-1.321	0.136	2.085	1.00	32.72
ATOM	489	CG	MET	1537	-2.282	1.208	1.566	1.50	37.18
ATOM	490	SD	MET	1537	-3.740	0.505	0.744	1.00	43.17
ATOM	491	CE	MET	1537	-2.964	-0 152	-0.698	1.00	43.04
ATOM	492	C	MET	1537	-0.903	-1.920	3.447	1.00	29.58
MOTA	493	C	MET	1537	-1.102	-3.049	2.996	1.00	27.63
MOTA	494	N	ILE	1538	0.142	-1.626	4.223	1.00	28.64
ATOM	495	CA	ILE	1538	1.189	-2.609	4.533	1.00	26.88
ATOM	496	CB	ILE	1538	2.381	-1.948	5.280	1.00	25.23
ATOM	497		ILE	1538	3.380	-2.989	5.745	1.00	27.31
MOTA	498	CG1	ILE	1538	3.097	-0.968	4.345	1.00	22.70
ATOM	499		ILE	153B	4.445	-0.465	4.874	1.00	23.44
ATOM	500	С	ILE	1538	0.756	-3.911	5.224	1.90	26.75
ATOM	501	0	ILE	1538	1.274	-4.980	4.909	1.00	28.60
ATOM	502	N	GLY	1539	-0.200	-3.849	6.137	1.00	27.19
ATOM	503	CA	GLY	1539	-0.625	-5.069	6.812	1.00	
ATOM	504	С	GLY	1539	0.207	-5.369	8.039	1.00	
ATOM	505	0	GLY	1539	1.220	-4.708	8.281	1.00	
MOTA	506	N	LYS	1540	-0.195	-6.396	8.788	1.00	23.25
ATOM	507	CA	LYS	1540	0.461	-6.781	10.052	1.00	
ATOM	508	CB	LYS	1540	-0.573	-7.350	11.028	1.00	
ATOM	509	CG	LYS	1540	-1.530	-6.346	11.563	1.00	
MOTA	510	CD	LYS	1540	-2.542	-6.977	12.502	1.00	36.24
MOTA	511	CE	LYS	1540	-3.568	-5.942	12.994	1.00	
ATOM	512	NZ	LYS	1540	-2.973	-4.847	13.836	1.00	
ATOM	513	С	LYS	1540	1.577	-7.796	9.974	1.00	
MOTA	514	0	LYS	1540	1.536	-8.723	9.176	1.00	21.51

ATOM	515	N	HIS	1541	2.514	~7.670	10.905	1.00 19.82
ATOM	516	CA	HIS	1541	3.622	-8.613	11.040	1.00 21.35
ATOM	517	СВ	HIS	1541	4.704	-8.411	9.972	1.00 21.39
ATOM	518	CG	HIS	1541	5. 74 7	-9.490	9.963	1.00 17.07
ATOM	519	CD2	HIS	1541	5.810	-10.667	9.292	1.00 18.04
MOTA	520	ND1	HIS	1541	6.891	-9.428	10.727	1.00 19.05
ATOM	521	CE1	HIS	1541	7.609	-10.522	10.535	1.00 19.63
MOTA	522	NE2	HIS	1541	6.975	-11.293	9.668	1.00 18.32
ATOM	523	C	HIS	1541	4.198	-8.456	12.449	1.00 23.61
ATOM	524	Ō	HIS	1541	4.231	-7.352	13.002	1.00 25.66
ATOM	525	N	LYS	1542	4.587	-9.577	13.045	1.00 24.32
ATOM	526	CA	LYS	1542	5.141	-9.610	14.396	1.00 27.04
ATOM	527.	CB	LYS	1542	5.578	-11.044	14.742	1.00.30.70
ATOM	528	CG	LYS	1542	6.130	-11.239	16.150	1.00 40.75
ATOM	529	CD	LYS	1542	6.380	-12.719	16.420	1.00 48.24
ATOM	530	CE	LYS	1542	6.995	-13.414	15.183	1.00 56.89
ATOM	531	NZ	LYS	1542	7.457	-14.831	15.421	1.00 60.99
MOTA	532	C	LYS	1542	. 6.318	-8.674	14.608	1.00 24.59
ATOM	533	0	LYS	1542	6.462	-8.067	15. 6 76	1.00 23.35
ATOM	534	N	ASN	1543	7.147	-8.546	13.576	1.00 22.05
MOTA	535	CA	ASN	1543	8.333	-7.702	13.689	1.00 21.40
ATOM	536	CB	ASN	1543	9.558	-8.482	13.217	1.00 20.89
MOTA	537	CG	ASN	1543	9.721	-9.811	13.945	1.00 20.37
MOTA	538	OD1	ASN	1543	9.501	-10.883	13.372	1.00 24.97
MOTA	539	ND2	ASN	1543	10.616	-9.741	15.230	1.00 21.56
MOTA	540	C	ASN	1543	8.312	-6.268	13.155	1.00 20.38
MOTA	541	0	ASN	1543	9.353	-5.733	12.776	1.00 20.03
ATOM	542	N	ILE	1544	7.153	-5.624	13.180	1.00 20.02
ATOM	543	CA	ILE	1544	7.037	-4.226	12.771	1.00 21.14
MOTA	544	CB	ILE	1544	6.545	-4.029	11.292	1.00 22.97
MOTA	545	CG2	ILE	1544	7.436	-4.810	10.334	1.00 23.27
MOTA	546	CG1	ILE	1544	5.082	-4.447	11.096	1.00 22.85
MOTA	547		ILE	1544	4.485	-3.974	9.760	1.00 18.94
ATOM	548	C	ILE	1544	6.044	-3.590	13.757	1.90 20.02
ATOM	549	0	ILE	1544	5.342	-4.309	14.466	1.00 21.00
ATOM	550	N	ILE	1545	6.103	-2.275	13.943	1.00 20.09
MOTA	551	CA	ILE	1545	5.140	-1.608	14.826	1.00 22.82
ATOM	552	CB	ILE	1545	5.586	-0.161	15.198	1.00 23.07
MOTA	553	CG2		1545	4.399	0.652	15.718	1.00 21.94
ATOM	554	CG1		1545	6.759	-0.178	16.193	1.00 20.49
MOTA	555	CD1		1545	6.450	-0.730	17.579	1.00 15.00
ATOM	556	C	ILE	1545	3.853	-1.555	14.010	1.00 24.18
ATOM	557	0	ILE	1545	3.809	-0.954	12.920	1.00 25.68
ATOM	558	N	ASN	1546	2.829	-2.236	14.514	1.00 25.69
ATOM	559	CA	ASN	1546	1.528	-2.311	13.853	1.00 24.23
ATOM	560	CB	ASN	1546	0.866	-3.697	14.060	1.00 25.21
ATOM	561	CG	ASN	1546	1.690	-4.834	13.481	1.00 21.10
ATOM	562	OD1		1546	1.764	-4.997	12.274	1.00 23.44
MOTA	563	ND2		1546	2.324	-5.606	14.343	1.00 18.20
ATOM	564	С	ASN	1546	0.567	-1.235	14.325	1.00 23.12
MOTA	565	0	ASN	1546	0.709	-0.682	15.426	1.00 24.14
ATOM	566	N	LEU	1547	-0.382	-0.920	13.456	1.00 23.49

ATOM	567	CA	LEU	1547	-1.417	0.069	13.718	1.00 24.50
ATOM	568	CB	LEU	1547	-1.976	0.597	12.378	1.00 21.63
ATOM	569	CG	LEU	1547	-3.189	1.535	12.353	1.00 22.37
ATOM	570	CD1	LEU	1547	-2.834	2.903	12.922	1.00 21.78
MOTA	571	CD2	LEU	1547	-3.714	1.660	10.930	1.00 21.31
MOTA	572	С	LEU	1547	-2.510	-0.681	14.495	1.00 26.70
MOTA	573	0	LEU	1547	-2.849	-1.823	14.160	1.00 28.96
MOTA	574	N	LEU	1548	-3.017	-0.082	15.565	1.00 25.96
ATOM	575	CA	LEU	1548	-4.047	-0.714	16.365	1.00 22.37
ATOM	576	CB	LEU	1548	-3.686	-0.682	17.868	1.00 17.76
ATOM	577	CG	LEU	1548	-2.346	-1.360	18.224	1.00 17.12
MOTA	578	CD1	LEU	1548	-2.150	-1.468	19.708	1.00 18.81
ATOM -	579	CD2	LEU	-1548	-2.266	-2.737	17.631	1.00 16.20
ATOM	580	С	LEU	1548	-5.395	-0.061	16.099	1.00 23.30
ATOM	581	0	LEU	1548	-6.418	-0.727	16.175	1.00 24.18
ATOM	582	N	GLY	1549	-5.395	1.228	15.758	1.00 21.53
MOTA	583	CA	GLY	1549	-6.636	1.933	15.485	1.00 22.47
ATOM	584	С	GLY	1549	-6.392	3.421	15.340	1.00 24.62
ATOM	585	0	GLY	1549	-5.245	3.835	15.163	1.00 25.06
ATOM	586	N	ALA	1550	-7.459	4.219	15.409	1.00 24.15
MOTA	587	CA	ALA	1550	-7.362	5.672	15.313	1.00 22.20
ATOM	588	CB	ALA	1550	-7.063	6.079	13.890	1.00 19.97
ATOM	589	С	ALA	1550	-8.602	6.415	15.802	1.00 23.75
ATOM	590	О	ALA	1550	-9.707	5.876	15.804	1.00 26.43
ATOM	591	N	CYS	1551	8.383	7.660	16.213	1.00 25.34
ATOM	592	CA	CYS	1551	-9.425	8.590	16.678	1.00 27.17
ATOM	593	CB	CYS	1551	-9.160	9.045	18.127	1.00 26.84
ATOM	594	SG	CYS	1551	-9.246	7.802	19.448	1.00 30.32
ATOM	595	C	CYS	1551	-9.294	9.787	15.719	1.00 28.42
ATOM	596	0	CYS	1551	-8.364	10.575	15.827	1.00 27.28
ATOM	597	N	THR	1552	10.145	9.823	14.702	1.00 30.47
ATOM	598	CA	THR	1552	-10.076	10.873	13.690	1.00 30.58
ATOM	599	CB	THR	1552	-10.061	10.219	12.290	1.00 30.58
ATOM	600	OG1 CG2	THR	1552	-11.266	9.465	12.096	1.00 31.11
ATOM ATOM	601		THR	1552	-8.895	9.255	12.151	1.00 27.59
ATOM	602 603	C 0	THR	1552	-11.241	11.847	13.695	1.00 32.24
ATOM	604	N	THR GLN	1552 1553	-11.192	12.911	13.070	1.00 28.56
ATOM	605	CA	GLN	1553	-12.339	11.408	14.286	1.00 35.46
ATOM	606	CB	GLN	1553	-13.529	12.233	14.295	1.00 38.72
ATOM	607	CG	GLN	1553	-14.775 -14.811	11.359	14.148	1.00 38.66
ATOM	608	CD	GLN	1553	-14.695	10.529	12.876	1.00 41.41
ATOM	609	OE1		1553	-14.693	11.381 12.345	11.627 11.445	1.00 44.05
ATOM	610	NE2	GLN	1553	-13.746	11.033	10.765	1.00 45.08 1.00 43.32
ATOM	611	C	GLN	1553	-13.658	13.168		1.00 43.32
ATOM	612	0	GLN	1553	-13.230	12.837	15.483 16.590	
ATOM	613	N	ASP	1554	-14.225	14.344	15.219	1.00 39.89 1.00 44.03
ATOM	614	CA	ASP	1554	-14.223	15.356	16.219	1.00 44.03
ATOM	615	СВ	ASP	1554	-15.778	15.028	16.237	1.00 46.94
ATOM	616	CG	ASP	1554	-13.778	15.026	16.122	1.00 49.94
ATOM	617		ASP	1554	-17.966	15.262	16.122	1.00 56.68
ATOM	618	OD2		1554	-17.030	14.829		
	0.10	UDZ	AUF	1004	-17.030	14.027	14.947	1.00 60.79

ATOM	619	C	ASP	1554	~13.343	15.563	17.244	1.00 47.24
ATOM	620	0	ASP	1554	-13.522	15.375	18.452	1.00 48.98
ATOM	621	N	GLY	1555	-12.182	15.966	16.747	1.00 44.00
ATOM	622	CA	GLY	1555	-11.062	16.185	17.638	1.00 41.07
MOTA	623	C	GLY	1555	-9.728	15.891	16.994	1.00 40.26
MOTA	624	0	GLY	1555	-9.663	15.567	15.810	1.00 39.72
MOTA	625	N	PRO	1556	-8.635	15.987	17.759	1.00 39.21
MOTA	626	CD	PRO	1556	-8.634	16.266	19.208	1.00 39.09
ATOM	627	CA	PRO	1556	-7.271	15.740	17.294	1.00 37.84
MOTA	628	CB	PRO	1556	-6.436	15.947	18.549	1.00 39.66
MOTA	629	CG	PRO	1556	-7.269	16.842	19.389	1.00 39.53
ATOM	630	С	PRO	1556	-7.094	14.314	16.806	1.00 37.75
ATOM	631	0	PRO	1556	7 574	13.377	17.444	1.00 37.25
MOTA	632	N	LEU	1557	-6.379	14.153	15.699	1.00 36.09
ATOM	633	CA	LEU	1557	-6.112	12.844	15.124	1.00 34.69
ATOM	634	СВ	LEU	1557	-5.458	13.010	13.741	1.00 32.25
ATOM	635	CG	LEU	1557	-4.962	11.774	12.972	1.00 31.23
ATOM	636		LEU	1557	-6.080	10.763	12.715	1.00 25.69
ATOM	637		LEU	1557	-4.339	12.219	11.669	1.00 28.21
ATOM	638	C	LEU	1557	-5.190	12.057	16.060	1.00 34.59
ATOM	639	Ö	LEU	1557	-4.173	12.578	16.524	1.00 32.09
ATOM	640	N	TYR	1558	-5.606	10.841	16.396	1.00 32.63
ATOM	641	CA	TYR	1558	-4.796	9.993	17.237	1.00 29.66
ATOM	642	СВ	TYR	1558	-5.529	9.633	18.534	1.00 33.14
ATOM	643	CG.	TYR	1558	-5.588	10.754	19.539	1.00 32.87
MOTA	644		TYR	1558	-6.583	10.793	20.517	1.00 34.58
ATOM	645	CE1		1558	-6.678	11.957	21.407	1.00 34.65
ATOM	646	CD2	TYR	1558	-4.678	11.805	19.483	1.00 35.69
ATOM	647	CE2		1558	-4.76C	12.878	20.367	1.00 37.03
ATOM	648	cz	TYR	1558	-5.766	12.899	21.324	1.00 37.52
ATOM	649	ОН	TYR	1558	-5.868	13.986	22.164	1.00 37.32
ATOM	650	C.	TYR	1558	-4.529	8.747	16.436	1.00 28.08
ATOM	651	0	TYR	1558	-5.467	8.137	15.924	1.00 30.12
ATOM	652	N	VAL	1559	-3.254	8.444	16.225	1.00 25 89
ATOM	653	CA	VAL	1559	-2.855	7.246	15.504	1.00 23.70
ATOM	654	СВ	VAL	1559	-1.729	7.528	14.485	1.00 23.78
ATOM	655		VAL	1559	-1.456	6.282	13 623	1.00 23.78
ATOM	656		VAL	1559	-2.101	8.738	13.604	1.00 20.75
ATOM	657	C	VAL	1559	-2.358	6.311	16.596	1.00 23.47
ATOM	658	ō	VAL	1559	-1.328	6.572	17.220	1.00 26.84
ATOM	659	N	ILE	1560	-3.146	5.283	16.889	
ATOM	660	CA	ILE	1560	-2.818	4.316	17.928	1.00 23.58 1.00 23.75
ATOM	661	СВ	ILE	1560	-4.112	3.732		
ATOM	662		ILE				18.552	1.00 22.67
ATOM	663	CG1		1560 1560	-3.777	2.898	19.788	1.00 20.24
ATOM					-5.063	4.884	18.904	1.00 20.09
ATOM	664	CD1		1560	-6.428	4.463	19.318	1.00 19.04
	665	C	ILE	1560	-1.954	3.181	17.356	1.00 27.39
ATOM	666	0	ILE	1560	-2.411	2.392	16.505	1.00 28.51
ATOM	667	N	VAL	1561	-0.720	3.089	17.840	1.00 26.76
ATOM	668	CA	VAL	1561	0.238	2.088	17.368	1.00 25.91
ATOM	669	CB	VAL	1561	1.445	2.801	16.653	1.00 24.50
ATOM	670	CG1	VAL	1561	0.952	3.480	15.397	1.00 13.55

ATOM	671	CG2	VAL	1561	2.054	3.870	17.551	1.00 20.39
MOTA	672	C	VAL	1561	0.693	1.151	18.519	1.00 24.80
MOTA	673	0	VAL	1561	0.397	1.417	19.696	1.00 25.26
MOTA	674	N	GLÜ	1562	1.349	0.032	18.192	1.00 22.30
MOTA	675	CA	GLU	1562	1.793	-0.901	19.230	1.00 21.49
ATOM	676	CB	GLU	1562	2.369	-2.179	18.630	1.00 16.65
ATOM	677	CG	GLU	1562	1.312	-3.115	18.092	1.00 19.71
ATOM	678	CD	GLU	1562	1.895	-4.356	17.460	1.00 21.58
ATOM	679	OE1	GLU	1562	1.281	-5.432	17.572	1.00 24.28
ATOM	680	OE2	GLU	1562	2.956	-4.260	16.825	1.00 23.74
ATOM	681	C	GLU	1562	2.802	0.261	20.158	1.00 23.56
MOTA	682	O .	GLU	1562	3.581	0.578	19.738	1.00 24.82
MOTA	683	N	TYR	1563 -	2.787	-0.665	21.422	1.00 26.96
ATOM	684	CA'	TYR	1563	3.677	-0 132	22.442	1.00 28.98
ATOM	685	CB	TYR	1563	2.907	0.035	23.744	1.00 30.34
ATOM	686	CG	TYR	1563	3.744	0.456	24.929	1.00 33,86
ATOM	687	CD1	TYR	1563	4.457	1.653	24.915	1.00 36.58
ATOM	688	CE1	TYR	1563	5.195	2.069	26.021	1.00 36.89
ATOM	689	CD2	TYR	1563	3.787	-0.322	26.082	1.00 34.25
ATOM	690	CE2	TYR	1563	4.522	0.080	27.186	1.00 34.47
MOTA	691	CZ	TYR	1563	5.219	1.273	27.150	1.00 37.08
ATOM	692	OH	TYR	1563	5.965	1.662	28.228	1.00 44.10
ATOM	693	C	TYR	1563	4.884	-1.043	22.668	1.00 30.53
MOTA	694	O	TYR	1563	4.745	-2.269	22.751	1.00 30.66
ATOM	695	Ŋ	ALA	1564	ອົ.068	-0.440	22.779	1.00 31.09
ATOM	696	CA	ALA	1564	7.303	-1.192	22.998	1.00 31.00
ATOM	697	CB	ALA	1564	8.236	-1.026	21.792	1.00 30.82
ATOM	698	C	ALA	1564	7.940	-0.663	24.283	1.00 25.32
ATOM	699	0	ALA	1564	8.703	0.309	24.274	1.00 32.26
ATOM	706	N	SER	1565	7.603	-1.303	25.389	1.00 29.55
ATOM	701	CA	SER	1565	8.059	-0.884	26.712	1.00 30.89
ATOM	702	CB	SER	1565	7.392	-1.729	27.792	1.00 29.79
ATOM ATOM	703	OG	SER	1565	7.704	-3.094	27.611	1.00 30.94
ATOM	704	C	SER	1565	9.547	-0.840	26.986	1.00 31.39
ATOM	705 706	O N	SER	1565	9.978	-0 150	27.902	1.00 35.74
MOTA	707	N CA	LYS	1566	10.340	-1.576	26.229	1.00 30.03
ATOM	708	CB	LYS	1566	11.756	-1.560	26.495	1.00 28.80
ATOM	709	CG	LYS LYS	1566	12.322	-2.973	26.447	1.00 28.98
ATOM	710	CD	LYS	1566 1566	11.756	-3.842	27.563	1.00 25.35
ATOM	711	CE	LYS	1566	12.208	-5.279	27.459	1.00 30.93
ATOM	712	NZ	LYS	1566	11.875	-6.001	28.747	1.00 31.41
ATOM	713	C	LYS	1566	12.315 12.529	-7.421	28.716	1.00 32.83
ATOM	714	0.	LYS	1566	13.756	-0.595	25.623	1.00 29.93
ATOM	715	N	GLY	1567	11.799	-0.672	25.544	1.00 30.89
ATOM	716	CA	GLY	1567	12.423	0.322	24.979	1.00 30.67
ATOM	717		GLY	1567	13.136	1.328	24.138	1.00 28.44
ATOM	718		GLY	1567	12.919	0.874	22.875	1.00 27.19
ATOM	719		ASN	1568	14.011	-0.235	22.395	1.00 25.36
ATOM	720		ASN	1568	14.011	1.731	22.352	1.00 28.39
ATOM	721		ASN	1568	14.735	1.421	21.130	1.00 28.41
ATOM	722	CG	ASN			2.698	20.418	1.00 30.32
	122	-0	HON	1568	16.396	3.352	21.058	1.00 33.42

ATOM	723	OD1	ASN	1568	17.418	2.720	21.317	1.00 35.16
MOTA	724	ND2	2 ASN	1568	16.328	4.661	21.203	1.00 36.23
MOTA	725	С	ASN	1568	15.884	0.443	21.314	1.00 28.34
ATOM	726	0	ASN	1568	16.478	0.373	22.388	1.00 30.67
ATOM	727	N	LEU	1569	16.212	-0.270	20.244	1.00 27.65
MOTA	728	CA	LEU	1569	17.269	-1.270	20.247	1.00 29.10
MOTA	729	CB	LEU	1569	17.311	-1.974	18.880	1.00 27.49
ATOM	730	CG	LEU	1569 .	18.292	-3.130	18.657	1.00 28.82
ATOM	731	CD1	LEU	1569	18.236	-4.140	19.825	1.00 24.68
MOTA	732	CD2	LEU	1569	17.994	-3.791	17.316	1.00 22.26
ATOM	733	C	LEU	1569	18.667	-0.790	20.676	1.00 29.37
ATOM	734	0	LEU	1569 .	19.389	-1.525	21.355	1.00 29.72
MOTA	735	N	ARG	1570	19.058	0.425	20.303	1.00 30.89
ATOM	736	CA	ARG	1570	20.374	0.943	20.689	1.00 33.01
ATOM	737	СВ	ARG	1.570	20.591	2.353	20.121	1.00 30.95
ATOM	738	CG	ARG	1570	21.896	2.983	20.584	1.00 38.85
ATOM	739	CD	ARG	1570	21.968	4.472	20.303	1.00 43.03
ATOM	740	NE	ARG	1570 .	20.749	5.192	20.670	1.00 53.34
ATOM	741	CZ	ARG	1570	20.404	5.573	21.905	1.00 57.49
ATOM	742	NH1	ARG	1570	21.184	5.310	22.955	1.00 55.59
ATOM	743	NH2	ARG	1570	19.272	6.252	22.086	1.00 59.53
ATOM	744	С	ARG	1570	20.475	0.947	22.229	1.00 33.82
ATOM	745	0	ARG	1570	21.351	0.296	22.817	1.00 33.93
MOTA	746	N	GLU	3.571	19.528	1.639	22.865	1.00 33.91
ATOM	747	CA	GLU	1571	19.435	1.746	24.317	1.00 32.59
ATOM	748	CB	GLU	1571	18.177	2.524	24.675	1.00 36.4C
MOTA	749	CG	GLU	1571	18.174	3.958	24.175	1.00 45.91
ATOM	750	CD	GLU	1571	16.822	4.654	24.328	1.00 52.95
ATOM	751	OE1	GLU	1571	15.793	3.959	24.529	1.00 54.50
ATOM	752		GLU	1571 .	16.792	5.905	24.222	1.00 55.17
ATOM	753	С	GLU	1571	19.380	0.361	24.959	1.00 31.40
MOTA	754	0	GLU	1571	20.115	0.054	25.895	1.00 31.09
ATOM	755	N	TYR	1.572	18.503	-0.477	24.433	1.00 29.24
ATOM	756	CA	TYR	1572	18.334	-1.835	24.920	1.00 27.43
ATOM	757	CB	TYR	1572	17.387	-2.590	23.991	1.00 26.41
ATOM	758	CG	TYR	1572 ·	17.196	-4.045	24.311	1.00 23.13
ATOM	759	CD1	TYR	1572	16.224	-4.448	25.216	1.00 28.16
ATOM	760	CEl	TYR	1572	15.983	-5.784	25.456	1.00 28.32
ATOM	761	CD2	TYR	1572	17.936	-5.024	23.665	1.00 20.00
MOTA	762	CE2	TYR	1572	17.699	-6.361	23.899	1.00 22.28
MOTA	763	CZ	TYR	1572	16.721	-6.731	24.801	1.00 26.53
ATOM	764	OH	TYR	1572	16.479	-8.058	25.055	1.00 30.25
ATOM	765	С	TYR	1572	19.671	-2.564	24.960	1.00 30.90
ATOM	766	0	TYR	1572	19.953	-3.323	25.901	1.00 30.68
ATOM	767	N	LEU	1573	20.487	-2.337	23.933	1.00 31.27
ATOM .	768	CA	LEU	1573	21.776	-2.995	23.841	1.00 33.33
ATOM	769	СВ	LEU	1573	22.287	-2.975	22.399	1.00 30.85
ATOM	770	CG	LEU	1573	21.643	-3.908	21.370	1.00 26.92
ATOM	771	CD1		1573	22.144	-3.546	19.980	1.00 22.76
ATOM	772	CD2		1573	21.939	-5.372	21.695	1.00 25.82
ATOM	773	С	LEU	1573	22.801	-2.390	24.791	1.00 36.07
ATOM	774	ō	LEU	1573	23.544	-3.117	25.457	1.00 36.40
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ATOM ATOM								
ATOM	775	N	GLN	1574	22.815	-1.065	24.887	1.00 37.25
	776	CA	GLN	1574	23.763	-0.391	25.759	1.00 37.41
MOTA	777	CB	GLN	1574	23.722	1.119	25.522	1.00 38.07
ATOM	778	CG	GLN	1574	24.240	1.529	24.147	1.00 40.76
ATOM	779	CD	GLN	1574	24.046	3.009	23.851	1.00 44.73
ATOM	780	OE1	GLN	1574	23.391	3.740	24.597	1.00 46.47
ATOM	781	NE2	GLN	1574	24.606	3.452	22.732	1.00 46.93
ATOM	782	C	GLN	1574	23.502	-0.711	27.233	1.00 37.80
ATOM	783	0	GLN	1574	24.431	-0.988	27.990	1.00 38.55
ATOM	784	N	ALA	1575	22.229	-0.742	27.617	1.00 37.28
MOTA	785	CA	ALA	1575	21.846	-1.021	28.987	1.00 35.47
MOTA	786	СВ	ALA	1575	20.394	-0.669	29.178	1.00 31.42
MOTA	787	- C	ALA	1575	22.102	-2.473	29.424	1:00 38.30
ATOM	788	0	ALA	1575	21.758	-2.843	30.544	1.00 41.11
MOTA	789	N	ARG	1576	22.647	~3.299	28.528	1.00 37.59
ATOM	790	CA	ARG	1576	22.943	-4.687	28.869	1.00 37.23
ATOM	791	CB	ARG	1576	22.027	-5.636	28.111	1.00 36.82
ATOM	792	CG	ARG	1576	20.599	-5.481	28.561	1.00 34.61
ATOM	793	CD	ARG	1.576	19.649	-6.146	27.640	1.00 31.82
ATOM	794	NE	ARG	1576	18.308	-6.147	28.201	1.00 31.54
ATOM	795	CZ	ARG	1576	17.590	-5.051	28.426	1.00 33.71
ATOM	796	NH1	ARG	1576	18.086	-3.855	28.149	1.00 33.68
MOTA	7 97	NH2	ARG	1576	16.337	-5.160	28.857	1.00 38.97
MOTA	798	С	ARG	1576	24.405	-5.052	28.683	1.00 38.53
MOTA	799	0	ARG	1576	24.790	-6.231	28.700	1.00 38.39
MOTA	800	N	ARG	1577	25.226	-4.017	28.538	1.00 39.28
ATOM	801	CA	ARG	1577	26.661	.4.185	28.394	1.00 39.33
MOTA	802	CB	ARG	1577	27.306	-2.855	27.998	1.00 35.44
ATOM	803	CG	ARG	1577	27.048	-2.402	26.584	1.00 33.45
ATOM	804	CD	ARG	1577	27.696	-1.042	26.330	1.00 32.83
MOTA	805	NE	ARG	1577	27.798	-0.747	24.897	1.00 36.69
3 moss								
MOTA	806	CZ	ARG	1577	28.284	0.385	24.384	1.00 36.99
MOTA	807	CZ NH1		1577 1577	28.284 28.719	0.385 1.359	24.384 25.175	1.00 36.99 1.00 40.35
ATOM ATOM		NH1 NH2						
MOTA MOTA MOTA	807	NH1	ARG ARG ARG	1577	28.719	1.359	25.175	1.00 40.35
MOTA MOTA MOTA	807 808	NH1 NH2	ARG ARG	1577 1577	28.719 28.346	1.359 0.539	25.175 23.065	1.00 40.35 1.00 36.53
MOTA MOTA MOTA MOTA	807 808 809 810 811	NH1 NH2 C O N	ARG ARG ARG ARG PRO	1577 1577 1577 1577 1578	28.719 28.346 27.222	1.359 0.539 -4.594	25.175 23.065 29.754 30.796 29.769	1.00 40.35 1.00 36.53 1.00 41.24
MOTA MOTA MOTA MOTA MOTA MOTA	807 808 809 810 811	NH1 NH2 C O N CD	ARG ARG ARG ARG PRO	1577 1577 1577 1577 1578	28.719 28.346 27.222 26.652	1.359 0.539 -4.594 -4.244	25.175 23.065 29.754 30.796	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03
MOTA MOTA MOTA MOTA MOTA MOTA MOTA	807 808 809 810 811 812 813	NH1 NH2 C O N CD CA	ARG ARG ARG PRO PRO PRO	1577 1577 1577 1577 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766	25.175 23.065 29.754 30.796 29.769 28.667 31.066	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	807 808 809 810 811 812 813	NH1 NH2 C O N CD CA CB	ARG ARG ARG PRO PRO PRO PRO	1577 1577 1577 1577 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	807 808 809 810 811 812 813 814	NH1 NH2 C O N CD CA CB	ARG ARG ARG PRO PRO PRO PRO PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 44.89
MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA	807 808 809 810 811 812 813 814 815	NH1 NH2 C O N CD CA CB CG	ARG ARG ARG PRO PRO PRO PRO PRO PRO PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817	NH1 NH2 C O N CD CA CB CG C	ARG ARG ARG PRO PRO PRO PRO PRO PRO PRO PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 44.68
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817	NH1 NH2 C O N CD CA CB CG C	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 44.68 1.00 46.51
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817 818	NH1 NH2 C O N CD CA CB CG C O N	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604 29.208	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432 -5.463	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003 33.981	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 44.68 1.00 46.51 1.00 46.36
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817 818 819	NH1 NH2 C O N CD CA CB CG C O N CD	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604 29.208 30.169	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432 -5.463 -3.265	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003 33.981 33.685	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 44.89 1.00 42.49 1.00 43.63 1.00 45.20 1.00 44.68 1.00 46.51 1.00 46.36 1.00 47.56
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817 818 819 820 821	NH1 NH2 C O CD CA CB CG C O N CD CA	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604 29.208 30.169 30.175	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432 -5.463 -3.265 -3.708	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003 33.981 33.685 35.141	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 46.51 1.00 46.36 1.00 47.56 1.00 46.45
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817 818 819 820 821	NH1 NH2 C O N CD CA CB CG O N CD CA CB	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604 29.208 30.169 30.175 28.997	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432 -5.463 -3.265 -3.708 -4.638	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003 33.981 33.685 35.141 35.205	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 46.51 1.00 46.36 1.00 47.56 1.00 47.56
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823	NH1 NH2 C O N CD CA CB CG C O N CD CA CB CG	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604 29.208 30.169 30.175 28.997 31.575	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432 -5.463 -3.265 -3.708 -4.638 -2.904	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003 33.981 33.685 35.141 35.205 33.200	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 46.51 1.00 46.36 1.00 47.56 1.00 47.56 1.00 47.51 1.00 50.19
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824	NH1 NH2 C O N CD CA CB CG O N CD CA CB CG C O	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604 29.208 30.169 30.175 28.997 31.575 32.481	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432 -5.463 -3.265 -3.708 -4.638 -2.904 -3.739	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003 33.981 33.685 35.141 35.205 33.200 33.196	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 46.51 1.00 46.36 1.00 47.56 1.00 47.56 1.00 47.51 1.00 50.19 1.00 53.53
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823	NH1 NH2 C O N CD CA CB CG C O N CD CA CB CG	ARG ARG ARG PRO	1577 1577 1577 1577 1578 1578 1578 1578	28.719 28.346 27.222 26.652 28.307 29.038 28.877 29.933 30.352 29.490 29.814 29.604 29.208 30.169 30.175 28.997 31.575	1.359 0.539 -4.594 -4.244 -5.381 -6.041 -5.766 -6.809 -6.391 -4.493 -3.538 -4.432 -5.463 -3.265 -3.708 -4.638 -2.904	25.175 23.065 29.754 30.796 29.769 28.667 31.066 30.686 29.327 31.672 30.947 33.003 33.981 33.685 35.141 35.205 33.200	1.00 40.35 1.00 36.53 1.00 41.24 1.00 41.03 1.00 44.39 1.00 44.50 1.00 42.49 1.00 43.63 1.00 45.20 1.00 46.51 1.00 46.36 1.00 47.56 1.00 47.56 1.00 47.51 1.00 50.19

ATOM	827	СВ	ALA	1592	20.975		33.715	1.00 61.58
ATOM	828	С	ALA	1592	21.367	-6.350	32.252	1.00 58.15
ATOM	829	0	ALA	1592	22.543	-6.285	31.879	1.00 59.09
ATOM	830	N	ALA	1593	20.754	~7.510	32.479	1.00 55.79
ATOM	831	CA	ALA	1593	21.457	-8.775	32.324	1.00 55.06
ATOM	832	CB	ALA	1593	20.519	-9.939	32.604	1.00 57.05
ATOM	833	С	ALA	1593	22.053	-8.897	30.924	1.00 53.57
ATOM	834	0	ALA	1593	21.402	-8.598	29.926	1.00 53.85
ATOM	835	N	GLN	1594	23.303	-9.336	30.862	1.00 53.22
ATOM	836	CA	GLN	1594	24.004	-9.490	29.599	1.00 50.13
ATOM	837	CB	GLN	1594	25.400	-10.082	29.832	1.00 50.73
ATOM	838	CG	GLN	1594	26.308		30.743	1.00 54.69
ATOM.	839.	CD	GLN	1594		-10.019	31.217	1.00 57.79
MOTA	840	OE1	GLN	1594	28.075	-10.900	30.524	1.00 58.82
ATOM	841	NE2	GLN	1594	28.026	-9.673	32.407	1.00 59.53
ATOM	842	С	GLN	1594		-10.374	28.637	1.00 47.73
ATOM	843	0	GLN	1594		-11.241	29.054	1.00 47.09
ATOM	844	N	LEU	1595		-10.133	27.350	1.00 45.64
ATOM	845	CA	LEU	1595		-10.880	26.292	1.00 42.00
ATOM	846	CB	LEU	1595	22.405	-9.947	25.122	1.00 37.98
MOTA	847	CG	LEU	1595	21.345	-8.894	25.446	1.00 37.70
ATOM	848	CD1	LEU	1595	21.568	7.611	24.660	1.00 33.34
ATOM	849	CD2	LEU	1.595	19.971	-9.479	25.222	1.00 32.84
ATOM	850	С	LEU	1595	23.729	-11.944	25.828	1.00 40.92
ATOM	851	0	LEU	1595		-11.745	25.855	1.00 41.12
ATOM	852	11	SER	1596		-13.103	25.471	1.00 40.09
ATOM	B 53	CA	SER	1596		-14.178	24.985	1.00 38.93
ATOM	854	CB	SER	1596		-15.535	25.235	1.00 37.45
MOTA	855	OG	SER	1596	22.158	-15.662	24.545	1.00 39.49
ATOM	856	C	SER	1596	24.302	-13.987	23.499	1.00 39.41
ATOM	857	0	SER	1596	23.634	-13.183	22.832	1.00 39.51
ATOM	858	N	SER	1597	25.266°	-14.738	22.977	1.00 39.17
ATOM	859	CA	SER	1597	25.587	-14.667	21.563	1.00 40.23
ATOM	860	CB	SER	1597	26.740	-15.611	21.230	1.00 39.96
ATOM	861	ЭG	SER	1597	27.865	-15.339	22.048	1.00 46.60
ATOM	862	2	SER	1597	24.347	-15.057	20.773	1.00 39.65
ATOM	863	0	SER	1597	24.066	-14.469	19.725	1.00 41.13
ATOM	864	N	LYS	1598	23.590	-16.023	21.291	1.00 36.82
MOTA	865	CA	LYS	1598	22.390	-16.467	20.611	1.00 36.17
MOTA	866	CB	LYS	1598	21.827	-17.742	21.217	1.00 36.19
ATOM	867	CG	LYS	1598	21.030	-18.562	20.180	1.00 39.59
ATOM	868	CD	LYS	1598	20.150	-19.623	20.830	1.00 37.49
ATOM	869	CE	LYS	1598	19.769	-20.719	19.855	1.00 39.64
ATOM	870	NZ	LYS	1598	20.976	-21.437	19.380	1.00 41.43
ATOM	871	С	LYS	1598		-15.381	20.649	1.00 37.72
ATOM	872	0	LYS	1598		-15.213	19.677	1.00 39.82
ATOM	B73	N	ASP	1599		-14.627	21.752	1.00 36.20
ATOM	874	CA	ASP	1599		-13.530	21.907	1.00 33.96
ATOM	875	СВ	ASP	1599		-12.884	23.279	1.00 35.66
ATOM	876	CG	ASP	1599		-13.744	24.394	1.00 36.18
ATOM	877		ASP	1599		-13.565	25.544	1.00 39.14
ATOM	878	OD2		1599		-14.593	24.128	1.00 33.40

ATOM	B 79	С	ASP	1599	20.595	-12.471	20.857	1.00 33.57
ATOM	880	0	ASP	1599	19.660	-11.953	20.225	1.00 32.60
MOTA	881	N	LEU	1600	21.871	-12.123	20.706	1.00 32.82
ATOM	882	CA	LEU	1600	22.304	-11.121	19.735	1.00 31.14
MOTA	883	CB	LEU	1600	23.804	-10.850	19.916	1.00 30.23
ATOM	884	CG	LEU	1600	24.174	-10.153	21.242	1.00 27.52
ATOM	885	CD1	LEU	1600	25.660	-9.877	21.324	1.00 24.11
MOTA	886	CD2	LEU	1600	23.408	-8.857	21.369	1.00 21.94
MOTA	887	С	LEU	1600	21.964	-11.523	18.291	1.00 29.24
MOTA	888	0	LEU	1600		-10.734	17.541	1.00 27.61
ATOM	889	N	VAL	1601	22.271	-12.764	17.930	1.00 27.38
ATOM	890	CA	VAL	1601	21.983	-13.268	16.597	1.00 27.26
ATOM	891	CB	VAL	1601	22.648	-14.649	16.345	1.00 30.47
ATOM	892	CG1	VAL	1601	22.403	-15.104	14.921	1.00 28.72
ATOM	893	CG2	VAL	1601	24.156	-14.568	16.593	1.00 29.92
ATOM	894	C	VAL	1601	20.474	-13.353	16.399	1.00 26.23
ATOM	895	0	VAL	1601	19.991	-13.147	15.295	1.00 25.54
ATOM	896	N	SER	1602	19.733	-13.590	17.478	1.00 27.43
ATOM	897	CA	SER	1602	18.277	-13.671	17.406	1.00 27.09
ATOM	898	СВ	SER	1602	17.731	-14.259	18.694	1.00 29.02
ATOM	899	OG	SER	1602	16.317	-14.306	18.646	1.00 35.77
ATOM	900	C	SER	1602	17.669	-12.280	17.149	1.00 26.87
MOTA	901	0	SER	1602	16.643	-12.141	16.465	1.00 25.13
ATOM	902	N	CYS	1603	18.289	-11.262	17.737	1.00 26.09
MOTA	903	CA	CYS	1603	17.878	-9.871	17.561	1.00 24.81
ATOM	904	CB	CYS	1603	18.797	-8.937	18.350	1.00 23.87
MOTA	905	SG	CYS	1603	18.512	-7.186	18.059	0.50 24.17
ATOM	906	С	CYS	1603	17.994	~9.517	16.090	1.00 25.24
ATOM	907	0	CYS	1603	17.083	-8.932	15.520	1.00 27.48
MOTA	908	N	ALA	1604	19.138	-9.854	15.492	1.00 26.80
MOTA	909	CA	ALA	1604	19.422	-9.592	14.073	1.00 26.15
MOTA	910	CB	ALA	1604	20.851	-10.035	13.741	1.00 24.35
MOTA	911	С	ALA	1604	18.419	-10.302	13.168	1.00 26.61
MOTA	912	0	ALA	1604	17.894	-9.713	12.226	1.00 28.81
MOTA	913	N	TYR	1605	18.130	-11.557	13.488	1.00 27.10
MOTA	914	CA	TYR	1605	17.175	-12.359	12.730	1.00 27.02
ATOM	915	CB	TYR	1605	17.104	-13.751	13.334	1.00 27.35
ATOM	916	CG	TYR	1605	15.997	-14.608	12.789	1.00 31.67
MOTA	917		TYR	1605		-15.244	11.546	1.00 32.96
MOTA	918		TYR	1605		-16.049	11.053	1.00 29.27
MOTA	919	CD2		1605		-14.797	13.520	1.00 31.42
ATOM	920		TYR	1605	13.801	-15.596	13.038	1.00 28.20
ATOM	921	CZ	TYR	1605		-16.212	11.810	1.00 29.20
MOTA	922	ОН	TYR	1605		-16.944	11.364	1.00 27.90
MOTA	923	С	TYR	1605		-11.735	12.658	1.00 27.90
MOTA	924	0.	TYR	1605		-11.635	11.578	1.00 28.40
ATOM	925	N	GLN	1606		-11.319	13.807	1.00 27.12
MOTA	926	CA	GLN	1606		-10.699	13.892	1.00 25.32
MOTA	927	CB	GLN	1606		-10.383	15.342	1.00 24.31
MOTA	928	CG	GLN	1606		-11.608	16.210	1.00 25.05
ATOM	929	CD	GLN	1606	13.052	-11.243	17.649	1.00 26.35
MOTA	930	OE1	GLN	1606	12.087	~10.542	17.944	1.00 26.11

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MOTA	931	NE2	GLN	1606	13.917	-11.684	18.551	1.00 27.77
ATOM	932	С	GLN	1606	13.849	-9.415	13.078	1.00 27.52
ATOM	933	0	GLN	1606	12.825	-9.089	12.455	1.00 27.87
ATOM	934	N	VAL	1607	14.943	-8.662	13.122	1.00 27.90
ATOM	935	CA	VAL	1607	15.053	-7.419	12.359	1.00 26.41
ATOM	936	CB	VAL	1607	16.337	-6.661	12.731	1.00 25.61
MOTA	937	CG1	VAL	1607	16.545	-5.457	11.800	1.00 27.37
ATOM	938	CG2	VAL	1607	16.277	-6.224	14.190	1.00 21.50
ATOM	939	С	VAL	1607	15.035	-7.718	10.860	1.00 26.09
ATOM	940	0	VAL	1607	14.337	-7.046	10.096	1.00 28.48
ATOM	941	N	ALA	1608	15.795	-8.722	10.435	1.00 23.05
ATOM	942	CA	ALA	1608	15.812	-9.079	9.027	1.00 20.32
ATOM	943	CB	ALA	1608	16.823	-10.145	8.783	1.00 14.95
ATOM	944	С	ALA	1608	14.418	-9.558	8.600	1.00 23.08
ATOM	945	0	ALA	1608	14.033	-9.405	7.432	1.00 23.91
ATOM	946	N	ARG	1609	13.671	-10.169	9.530	1.00 24.57
ATOM	947	CA	ARG	1609	12.314	-10.628	9.246	1.00 24.30
ATOM	948	СВ	ARG	1609	11.822	-11.577	10.326	1.00 26.13
ATOM	949	CG	ARG	1609	12.278	-12.979	10.114	1.00 31.07
ATOM	950	CD	ARG	1609	11.449	-13.885	10.939	1.00 36.13
ATOM	951	NE	ARG	1609	10.771	-14.865	10.115	1.00 38.37
ATOM	952	CZ	ARG	1609	9.931	-15.778	10.594	1.00 37.95
ATOM	953	NHl	ARG	1609	9.674	-15.828	11.898	1.00 35.31
ATOM	954	NH2	ARG	1609	9.353	-16.649	9.776	1.00 37.85
MOTA	955	С	ARG	1609	11.318	-9.490	9.065	1.00 22.34
MOTA	956	0	ARG	1609	10.470	-9.542	8.160	1.00 24.57
ATOM	957	N	GLY	1610	11.375	-8.500	9.948	1.00 20.52
ATOM	958	CA	GLY	1610	10.497	-7.353	9.827	1.00 19.33
ATOM	959	С	GLY	1610	10.732	-6.715	8.464	1.00 20.04
ATOM	960	0	GLY	1610	9.794	-6.455	7.693	1.00 19.10
ATOM	961	N	MET	1611	12.011	-6.545	8.130	1.00 18.21
ATOM	962	CA	MET	1611	12.423	-5.970	6.851	1.00 20.32
ATOM	963	CB	MET	1611	13.925	-5.737	6.838	1.00 19.20
ATOM	964	CG	MET	1611	14.371	-4.547	7.694	1.00 20.83
MOTA	965	SD	MET	1611	13.449	-2.960	7.422	1.00 25.39
MOTA	966	CE	MET	1611	13.869	-2.525	5.757	1.00 18.67
ATOM	967	С	MET	1611	12.024	-6.843	5.670	1.00 23.98
ATOM	968	0	MET	1611	11.608	-6.332	4.613	1.00 24.13
MOTA	969	N	GLU	1612	12.141	-8.162	5.825	1.00 25.76
MOTA	970	CA	GLU	1612	11.759	-9.059	4.743	1.00 25.49
MOTA	971	CB	GLU	1612	11.980	-10.522	5.110	1.00 26.09
ATOM	972	CG	GLU	1612	11.587	-11.468	3.968	1.00 26.56
ATOM	973	CD	GLU	1612	11.735	-12.942	4.313	1.00 29.26
ATOM	974	OE1	GLU	1612	11.386	-13.316	5.448	1.00 29.10
ATOM	975	OE2	GLU	1612	12.190	-13.725	3.443	1.00 31.11
ATOM	976	С	GLU	1612	10.283	-8.821	4.398	1.00 26.29
MOTA	977	0	GLU	1612	9.916	-8.728	3.226	1.00 28.46
MOTA	978	N	TYR	1613	9.437	-8.700	5.422	1.00 24.78
ATOM	979	CA	TYR	1613	8.003	-8.456	5.212	1.00 23.07
MOTA	980	СВ	TYR	1613	7.263	-8.526	6.549	1.00 23.75
MOTA	981	CG	TYR	1613	5.785	-8.218	6.449	1.00 20.80
ATOM	982	CD1		1613	4.880	-9.213	6.062	1.00 20.97

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ATOM	983	CE1	TYR	1613	3.517	-8.944	5.958	1.00 20.03
MOTA	984	CD2	TYR	1613	5.289	-6.938	6.731	1.00 19.72
MOTA	985	CE2	TYR	1613	3.926	-6.661	6.628	1.00 21.87
MOTA	986	CZ	TYR	1613	3.046	-7.672	6.244	1.00 24.87
ATOM	987	OH	TYR	1613	1.694	-7.420	6.161	1.00 24.37
MOTA	988	C	TYR	1613	7.766	-7.094	4.550	1.00 21.68
ATOM	989	0	TYR	1613	6.970	-6.979	3.615	1.00 20.20
MOTA	990	N	LEU	1614	8.436	-6.065	5.062	1.00 21.72
ATOM	991	CA	LEU	1614	8.321	-4.713	4.519	1.00 20.42
ATOM	992	CB	LEU	1614	9.169	-3.747	5.350	1.00 17.68
ATOM	993	CG	LEU	1614	8.607	-3.395	6.733	1.00 18.47
MOTA	994	CD1	LEU	16Ì4	9.504	-2.425	7.470	1.00 16.59
MOTA	995	CD2	LEU	1614	7.230	-2.795	···6.558	1.00 14.07
MOTA	996	C	LEU	1614	8.729	-4.676	3.043	1.00 21.70
ATOM	997	0	LEU	1614	8.073	-4.038	2.211	1.00 22.25
ATOM	998	N	ALA	1615	9.819	-5.366	2.729	1.00 21.55
ATOM	999	CA	ALA	1615	10.313	-5.435	1.355	1.00 20.52
MOTA	1000	CB	ALA	1615	11.625	-6.207	1.292	1.00 19.78
ATOM	1001	С	ALA	1615	9.264	-6.098	0.491	1.00 19.98
MOTA	1002	0	ALA	1615	8.945	-5.587	-0.579	1.00 20.14
MOTA	1003	N	SER	1616	8.692	-7.205	0.972	1.00 20.65
MOTA	1004	CA	SER	1616	7.660	-7.919	0.207	1.00 19.59
MOTA	1005	CB	SER	1616	7.283	-9.217	0.912	1.00 15.96
ATOM	1006	OG	SER	1616	6.415	-8.966	2.007	1.00 16.62
ATOM	1007	С	SER	1616	6.397	-7.062	-0.018	1.00 22.05
MOTA	1008	0	SER	1616	5.650	-7.266	-0.975	1.00 23.62
ATOM	1009	N	LYS	1617	6.136	-6.135	0.895	1.00 23.39
ATOM	1010	CA	LYS	1617	4.997	-5.237	0.779	1.00 23.02
MOTA	1011	CB	LYS	1617	4.436	-4.881	2.160	1.00 21.50
ATOM	1012	CG	LYS	1617	3.709	-6.046	2.851	1.00 24.94
ATOM	1013	CD	LYS	1617	2.463	-6.448	2.059	1.00 26.57
MOTA	1014	CE	LYS	1617	1.691	-7.571	2.725	1.00 31.05
ATOM	1015	NZ	LYS	1617	2.401	-8.852	2.601	1.00 38.73
ATOM	1016	С	LYS	1617	5.346	-3.981	-0.017	1.00 24.01
ATOM	1017	0	LYS	1617	4.588	-3.007	-0.013	1.00 28.15
MOTA	1018	N	LYS	1618	6.496	-4.002	-0.679	1.00 23.84
ATOM	1019	CA	LYS	1618	6.957	~2.883	-1.528	1.00 24.05
ATOM	1020	CB	LYS	1618	5.871	-2.513	-2.555	1.00 25.74
MOTA	1021	CG	LYS	1618	5.734	-3.465	-3.749	1.00 28.34
MOTA	1022	CD	LYS	1618	5.557	-4.914	-3.328	1.00 32.45
MOTA	1023	CE	LYS	1618	5.590	-5.850	-4.520	1.00 30.41
ATOM	1024	NZ	LYS	1618	4.373	-5.748	-5.354	1.00 31.84
MOTA	1025	С	LYS	1618	7.404	-1.610	-0.796	1.00 23.84
ATOM	1026	0	LYS	1618	7.533	-0.548	-1.402	1.00 20.60
ATOM	1027	N	CYS	1619	7.719	-1.744	0.489	1.00 25.11
MOTA	1028	CA	CYS	1619	8.103	-0.614	1.312	1.00 21.68
ATOM	1029	CB	CYS	1619	7.338	-0.690	2.643	1.00 20.84
ATOM	1030	SG	CYS	1619	7.916	0.427	3.957	1.00 26.69
MOTA	1031	С	CYS	1619	9.586	-0.480	1.543	1.00 23.16
ATOM	1032	0	CYS	1619	10.257	-1.435	1.958	1.00 25.60
ATOM	1033	N	ILE	1620	10.110	0.717	1.288	1.00 23.91
ATOM	1034	CA	ILE	1620	11.532	1.046	1.474	1.00 26.01

ATOM	1035	CB	ILE	1620	12.098	1.830	0.236	1.00 22.61
ATOM	1036	CG2	ILE	1620	13.551	2.259	0.471	1.00 16.86
MOTA	1037	CG1	ILE	1620	12.014	0.977	-1.026	1.00 22.72
ATOM	1038	CD1	ILE	1620	12.096	1.804	-2.316	1.00 23.62
MOTA	1039	C	ILE	1620	11.566	1.934	2.729	1.00 26.83
MOTA	1040	0	ILE	1620	10.900	2.965	2.772	1.00 28.92
MOTA	1041	N	HIS	1621	12.293	1.500	3.758	1.00 26.44
MOTA	1042	CA	HIS	1621	12.386	2.245	5.007	1.00 23.61
MOTA	1043	CB	HIS	1621	13.142	1.429	6.065	1.00 20.98
ATOM	1044	CG	HIS	1621	12.940	1.917	7.463	1.00 21.57
ATOM	1045	CD2	HIS	1621	12.321	1.346	8.528	1.00 20.74
ATOM	1046	ND1	HIS	1621	13.382	3.151	7.897	1.00 21.08
- ATOM -	1.047	CE1	HIS	1621	13.035	3.321	9.162	1.00 21.00
ATOM	1048	NE2	HIS	1621	12.396	2.237	9.572	1.00 21.97
ATOM	1049	С	HIS	1621	13.054	3.582	4.841	1.00 24.83
MOTA	1050	0	HIS	1621	12.560	4.585	5.310	1.00 25.76
ATOM	1051	N	ARG	1622	14.247	3.565	4.269	1.00 27.57
ATOM	1052	CA	ARG	1622	15.056	4.776	4.066	1.00 26.47
ATOM	1053	СВ	ARG	1622	14.233	5.918	3.460	1.00 20.08
MOTA	1054	CG	ARG	1622	13.762	5.634	2.077	1.00 15.87
ATOM	1055	CD	ARG	1622	12.998	6.791	1.501	0.50 11.86
ATOM	1056	NE	ARG	1622	12.613	6.458	0.144	0.50 12.46
ATOM	1057	CZ	ARG	1622	11.537	5.748	-0.178	0.50 11.18
ATOM	1058	NHl	ARG	1622	10.711	5.304	0.767	0.50 7.16
ATOM .	1059	NH2	ARG	1622	11.340	5.398	-1.442	0.50 9.57
ATOM	1060	С	ARG	1622	15.813	5.250	5.325	1.00 26.18
ATOM	1061	0	ARG	1622	16.645	6.150	5.250	1.00 26.90
ATOM	1062	N	ASP	1623	15.544	4.650	6.480	1.00 27.26
ATOM	1063	CA	ASP	1623	16.268	5.042	7.684	1.00 29.80
ATOM	1064	CB	ASP	1623	15.714	6.330	8.292	1.00 32.13
MOTA	1065	CG	ASP	1623	16.690	6.940	9.298	1.00 37.87
MOTA	1066	OD1	ASP	1623	16.237	7.671	10.202	1.00 42.95
MOTA	1067	OD2	ASP	1623	17.907	6.684	9.191	1.00 41.09
ATOM	1068	С	ASP	1623	16.364	3.943	8.738	1.00 29.10
ATOM	1069	0	ASP	1623	16.164	4.168	9.939	1.00 27.69
ATOM	1070	N	LEU	1624	16.723	2.755	8.270	1.00 28.23
MOTA	1071	CA	LEU	1624	16.874	1.599	9.129	1.00 26.00
ATOM	1072	CB	LEU	1624	16.944	0.351	8.245	1.00 22.14
ATOM	1073	CG	LEU	1624	17.036	-0.998	8.941	1.00 22.32
ATOM	1074	CD1	LEU	1624	15.853	-1.196	9.932	1.00 17.01
ATOM	1075	CD2	LEU	1624	17.068	-2.064	7.848	1.00 20.50
ATOM	1076	С	LEU	1624	18.129	1.757	10.003	1.00 25.89
ATOM	1077	0	LEU	1624	19.247	1.917	9.499	1.00 26.11
ATOM	1078	N	ALA	1625	17.930	1.706	11.316	1.00 25.58
MOTA	1079	CA	ALA	1625	19.006	1.864	12.292	1.00 23.16
ATOM	1080	СВ	ALA	1625	19.323	3.340	12.493	1.00 19.06
ATOM	1081	С	ALA	1625	18.475	1.286	13.584	1.00 24.12
ATOM	1082	0	ALA	1625	17.269	1.083	13.721	1.00 27.40
ATOM	1083	N	ALA	1626	19.357	1.041	14.543	1.00 24.67
ATOM	1084	CA	ALA	1626	18.929	0.491	15.827	1.00 25.07
ATOM	1085	СВ	ALA	1626	20.148	0.145	16.691	1.00 26.06
ATOM	1086	С	ALA	1626	18.015	1.474	16.560	1.00 25.13

ATOM	1087	O	ALA	1626	17.184	1.069	17.366	1.00 26.38
ATOM	1088	N	ARG	1627	18.197	2.770	16.308	1.00 23.08
ATOM	1089	CA	ARG	1627	17.367	3.784	16.939	1.00 24.05
MOTA	1090	CB	ARG	1627	17.850	5.187	16.565	1.00 28.05
ATOM	1091	CG	ARG	1627	17.731	5.501	15.078	1.00 37.58
ATOM	1092	CD	ARG	1627	18.159	6.920	14.740	1.00 42.10
ATOM	1093	NE	ARG	1627	18.448	7.085	13.310	1.00 42.67
ATOM	1094	CZ	ARG	1627	19.667	7.006	12.784	1.00 43.58
MOTA	1095		ARG	1627	20.717	6.752	13.561	1.00 46.17
MOTA	1096	NH2	ARG	1627	19.841	7.201	11.492	1.00 43.78
ATOM	1097	C	ARG	1627	15.926	3.632	16.482	1.00 23.04
ATOM	1098	0	ARG	1627	15.015	3.979	17.216	1.00 22.27
MOTA	1099	N	ASN	1628	15.722	3.093	15.286	1.00 24.49
MOTA	1100	CA	ASN	1628	14.382	2.934	14.723	1.00 23.80
MOTA	1101	CB	ASN	1628	14.351	3.407	13.269	1.00 27.82
ATOM	1102	CG	ASN	1628	14.503	4.918	13.143	1.00 30.25
ATOM	1103	OD1	ASN	1628	13.876	5.686	13.863	1.00 32.33
MOTA	1104	ND2	ASN	1628	15.361	5.348	12.220	1.00 31.50
MOTA	1105	C	ASN	1628	13.782	1.524	14.833	1.00 23.93
ATOM	1106	0	ASN	1628	12.896	1.161	14.056	1.00 23.64
MOTA	1107	N	VAL	1629	14.307	0.733	15.763	1.00 24.10
ATOM	1108	CA	VAL	1629	13.778	-0.610	16.036	1.00 22.59
ATOM	1109	CB	VAL	1629	14.829	-1.727	15.823	1.00 21.16
ATOM	1110		VAL	1629	14.346	-3.014	16.462	1.00 17.53
ATOM	1111	CG2	VAL	1629	15.068	-1.962	14.341	1.00 14.48
MOTA	1112	С	VAL	1629	13.411	-0.575	17.520	1.00 24.81
ATOM	1113	0	VAL	1629	14.237	-0.204	18.357	1.00 24.09
ATOM	1114	N	LEU	1630	12.181	-0.941	17.850	1.00 24.34
ATOM	1115	CA	LEU	1630	11.751	-0.919	19.239	1.00 26.53
ATOM	1116	CB	LEU	1630	10.447	-0.129	19.359	1.00 26.19
ATOM	1117	CG	LEU	1630	10.522	1.293	18.758	1.00 24.33
ATOM	1118		LEU	1630	9.149	1.870	18.601	1.00 20.51
ATOM	1119		LEU	1630	11.339	2.196	19.618	1.00 19.77
ATOM	1120	C	LEU	1630	11.641	-2.327	19.835	1.00 28.14
ATOM	1121	0	LEU	1630	11.475	-3.320	19.108	1.00 28.31
ATOM	1122	N	VAL	1631	11.792	-2.418	21.153	1.00 28.21
ATOM	1123	CA	VAL	1631	11.741	-3.694	21.866	1.00 26.96
ATOM	1124	CB	VAL	1631	13.068	-3.930	22.624	1.00 25.71
ATOM	1125	CG1		1631	13.113	-5.345	23.222	1.00 20.40
ATOM	1126	CG2		1631	14.240	-3.688	21.680	1.00 19.88
ATOM	1127	C	VAL	1631	10.560	-3.758	22.836	1.00 29.84
ATOM	1128	0	VAL	1631	10.419	-2.918	23.738	1.00 32.46
ATOM	1129	N	THR	1632	9.703	-4.756	22.641	1.00 30.90
ATOM	1130	CA	THR	1632	8.530	-4.939	23.487	1.00 31.16
	1131	CB	THR	1632	7.476	-5.800	22.793	1.00 29.58
ATOM	1132	OG1		1632	7.948	-7.152	22.708	1.00 29.17
ATOM	1133		THR	1632	7.186	-5.262	21.414	1.00 22.23
ATOM	1134	C	THR	1632	8.882	-5.603	24.809	1.00 32.23
ATOM	1135	0	THR	1632	9.950	-6.185	24.946	1.00 33.23
ATOM	1136	N	GLU	1633	7.946	-5.589	25.751	1.00 34.38
ATOM	1137	CA	GLU	1633	8.165	-6.193	27.062	1.00 35.51
ATOM	1138	CB	GLU	1633	6.881	-6.114	27.899	1.00 35.48

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ATOM	1139	CG	GLU	1633	7.004	-6.685	29.309	1.00 45.	16		
ATOM	1140	CD	GLU	1633	8.070	-5.999	30.183	1.00 50.	15		
MOTA	1141	OE1	GLU	1633	8.174	-4.750	30.163	1.00 52.	70		
ATOM	1142	OE2	GLU	1633	8.789	-6.723	30.919	1.00 53.	59		
MOTA	1143	С	GLU	1633	8.624	-7.635	26.930	1.00 35.4	10		
ATOM	1144	0	GLU	1633	9.387	-8.119	27.758	1.00 36.9			
ATOM	1145	N	ASP	1634	8.204	-8.308	25.861	1.00 36.			
ATOM	1146	CA	ASP	1634	8.573	-9.709	25.662	1.00 37.9			
MOTA	1147	CB	ASP	1634	7.435	-10.491	24.991	1.00 42.9			
MOTA	1148	CG	ASP	1634	6.100	-10.315	25.706	1.00 49.0			
ATOM	1149	OD1	ASP	1634	5.885	-10.957	26.759	1.00 50.9	5		
ATOM	1150	OD2	ASP	1634	5.256	-9.544	25.197	1.00 53.9			
ATOM	1151	·C	ASP	1634	9.842	-9.882	24.840	1.00 36.0		;	
ATOM	1152	0	ASP	1634	10.148	-10.988	24.414	1.00 34.9			
ATOM	1153	N	ASN	1635	10.582	-8.787	24.655	1.00 36.5		•	
ATOM	1154	CA	ASN	1635	11.833	-8.763	23.868	1.00 36.2			
ATOM	1155	CB	ASN	1635	12.893	-9.692	24.471	1.00 37.9			
ATOM	1156	CG	ASN	1635	13.335	-9.244	25.840	1.00 37.6	0		
MOTA	1157	OD1	ASN	1635	13.496	-8.057	26.088	1.00 42.7	2		
MOTA	1158	ND2	ASN	1635	13.525	-10.191	26.743	1.00 38.0			
ATOM	1159	C	ASN	1635	11.641	-9.073	22.372	1.00 34.5	9		
ATOM	1160	0	ASN	1635	12.431	-9.799	21.754	1.00 33.5	2		
ATOM	1161	N	VAL	1636	10.557	-8.541	21.819	1.00 31.9	5		
MOTA	1162	CA	VAL	1636	10.260	-8.722	20.415	1.00 28.9			
ATOM	1163	CB	VAL	1636	8.743	-8.945	20.177	1.00 31.0	0		
MOTA	1164	CG1	VAL	1636	8.451	-9.066	18.678	1.00 29.5	2		
MOTA	1165	CG2	VAL	1636	8.289	-10.220	20.884	1.00 29.0	3		
ATOM	1166	С	VAL	1636	10.725	-7.461	19.721	1.00 28.0	5		
ATOM	1167	0	VAL	1636	10.432	-6.355	20.179	1.00 25.2	1		
ATOM	1168	И	MET	1637	. 11.567	-7.637	18.707	1.00 28.7	8		
MOTA	1169	CA	MET	1637	12.107	-6.539	17.927	1.00 27.2	9		
MOTA	1170	CB	MET	1637	13.325	-7.008	17.138	1.00 27.9	7		
MOTA	1171	CG	MET	1637	14.446	-7.576	17.982	1.00 29.3	1		
MOTA	1172	SD	MET	1637	15.051	-6.440	19.245	1.00 29.5	8		
ATOM	1173	CE	MET	1637	15.163	-7.542	20.648	1.00 23.5	1		
ATOM	1174	C	MET	1637	11.033	-6.108	16.951	1.00 26.6	0		
ATOM	1175	0	MET	1637	10.479	-6.951	16.244	1.00 26.6	0		
ATOM	1176	N	LYS	1638	10.758	-4.805	16.893	1.00 24.3	5		
ATOM	1177	CA	LYS	1638	9.745	-4.255	16.006	1.00 20.7			
MOTA	1178	CB	LYS	1638	8.495	-3.883	16.793	1.00 18.9			
ATOM	1179	CG	LYS	1638	7.723	-5.087	17.268	1.00 22.8	2		
ATOM	1180	CD	LYS	1638	6.442	-4.699	17.969	1.00 25.4	9		
ATOM	1181		LYS	1638	5.560	-5.934	18.189	1.00 24.3			
ATOM	1182		LYS	1638	4.892	-6.414	16.941	1.00 22.2			
ATOM	1183		LYS	1638	10.254	-3.034	15.257	1.00 22.7			
ATOM	1184		LYS	1638	10.613	-2.041	15.868	1.00 24.6)		
ATOM	1185	N	ILE	1639	10.259	-3.101	13.934	1.00 23.9			
ATOM	1186		ILE	1639	10.707	-1.984	13.113	1.00 24.2			
ATOM	1187		ILE	1639	10.925	-2.439	11.648	1.00 23.1			
ATOM	1188	CG2		1639	11.270	-1.262	10.766	1.00 17.1			
ATOM	1189	CG1		1639	12.068	-3.454	11.604	1.00 19.9			
ATOM	1190	CD1	ILE	1639	11.975	-4.369	10.461	1.00 26.9	2		

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ATOM	1191	С	ILE	1639	9.686	-0.846	13.173	1.00 25.63
MOTA	1192	0	ILE	1639	8.473	-1.075	13.042	1.00 26.20
ATOM	1193	N	ALA	1640	10.200	0.364	13.390	1.00 27.31
ATOM	1194	CA	ALA	1640	9.394	1.577	13.497	1.00 27.45
ATOM	1195	CB	ALA	1640	9.623	2.211	14.862	1.00 27.20
MOTA	1196	C	ALA	1640	9.720	2.595	12.411	1.00 27.87
ATOM	1197	0	ALA	1640	10.765	2.522	11.755	1.00 26.95
MOTA	1198	N	ASP	1641	8.815	3.551	12.237	1.00 29.66
MOTA	1199	CA	ASP	1641	8.952	4.631	11.259	1.00 31.25
ATOM	1200	CB	ASP	1641	10.096	5.581	11.646	1.00 33.40
ATOM	1201	CG	ASP	1641	9.713	6.551	12.771	1.00 33.86
ATOM	1202	OD1	ASP	1641	10.475	7.524	12.953	1.00 37.57
ATOM	1203	OD2	ASP	1641	8.684	6.355	13.470	1.00 29.83
ATOM	1204	С	ASP	1641	9.088	4.228	9.799	1.00 30.77
ATOM	1205	0	ASP	1641	9.526	5.022	8.966	1.00 29.52
ATOM	1206	N	PHE	1642	8.611	3.032	9.477	1.00 30.38
ATOM	1207	CA	PHE	1642	8.664	2.528	8.114	1.00 29.43
MOTA	1208	CB	PHE	1642	8.459	1.009	8.100	1.00 25.46
ATOM	1209	CG	PHE	1642	7.167	0.555	8.697	1.00 20.44
ATOM	1210	CD1	PHE	1642	6.002	0.547	7.942	1.00 22.76
ATOM	1211	CD2	PHE	1642	7.119	0.112	10.007	1.00 18.52
ATOM	1212	CEI	PHE	1642	4.796	0.094	8.485	1.00 25.55
ATOM	1213	CE2	PHE	1642	5.926	-0.341	10.559	1.00 21.76
ATOM	1214	CZ	PHE	1642	4.760	-0.352	9.802	1.00 24.94
ATOM	1215	С	PHE	1642	7.686	3.242	7.163	1.00 31.03
MOTA	1216	0	PHE	1642	7.946	3.330	5.975	1.00 35.19
MOTA	1217	N	GLY	1643	6.600	3.791	7.693	1.00 30.42
ATOM	1218	CA	GLY	1643	5.640	4.476	6.845	1.00 28.27
MOTA	1219	C	GLY	1643	5.736	5.991	6.874	1.00 28.46
ATOM	1220	0	GLY	1643	4.896	6.707	6.332	1.00 24.29
ATOM	1221	N	LEU	1644	6.816	6.471	7.458	1.00 31.65
ATOM	1222	CA	LEU	1644	7.077	7.890	7.601	1.00 36.03
ATOM	1223	CB	LEU	1644	8.363	8.058	8.389	1.00 32.41
MOTA	1224	CG	LEU	1644	8.321	9.137	9.446	1.00 35.30
ATOM	1225	CD1	LEU	1644	7.161	8.827	10.384	1.00 37.60
ATOM	1226	CD2	LEU	1644	9.663	9.186	10.190	1.00 36.62
ATOM	1227	C	LEU	1644	7.178	8.708	6.293	1.00 40.21
MOTA	1228	0	LEU	1644	7.770	8.267	5.312	1.00 40.65
ATOM	1229	N	ALA	1645	6.553	9.881	6.293	1.00 44.50
ATOM	1230	CA	ALA	1645	6.591	10.786	5.148	1.00 48.66
MOTA	1231	CB	ALA	1645	5.432	11.762	5.241	1.00 45.63
ATOM	1232	С	ALA	1645	7.935	11.545	5.173	1.00 51.32
MOTA	1233	0	ALA	1645	8.254	12.200	6.163	1.00 52.68
ATOM	1234	N	ALA	1646	8.727	11.444	4.107	1.00 52.77
ATOM	1235	CA	ALA	1646	10.023	12.121	4.077	1.00 54.73
ATOM	1236	CB	ALA	1646	11.108	11.194	4.646	1.00 55.34
MOTA	1237	C	ALA	1646	10.446	12.601	2.692	1.00 56.41
MOTA	1238	0	ALA	1646	10.430	11.823	1.740	1.00 57.76
MOTA	1239	N	ASP	1647	10.811	13.876	2.567	1.00 58.20
MOTA	1240	CA	ASP	1647	11.280	14.394	1.283	1.00 59.39
MOTA	1241	СВ	ASP	1647	10.898	15.861	1.083	1.00 59.29
MOTA	1242	CG	ASP	1647	11.128	16.339	-0.356	1.00 60.67

ATOM	1243	OD1	ASP	1647	12.110	15.908	-1.009	1.00 61.21
MOTA	1244	OD2	ASP	1647	10.337	17.173	-0.835	1.00 61.34
MOTA	1245	C	ASP	1647	12.793	14.236	1.273	1.00 60.16
ATOM	1246	0	ASP	1647	13.523	15.023	1.889	1.00 58.16
MOTA	1247	N	ILE	1648	13.248	13.209	0.562	1.00 61.28
MOTA	1248	CA	ILE	1648	14.658	12.878	0.439	1.00 62.12
MOTA	1249	CB	ILE	1648	14.848	11.626	-0.444	1.00 59.97
ATOM	1250	CG2	ILE	1648	14.023	10.469	0.131	1.00 58.26
ATOM	1251	CG1	ILE	1648	14.429	11.922	-1.883	1.00 55.69
ATOM	1252	CD1	ILE	1648	15.005	10.976	-2.890	1.00 54.38
ATOM	1253	C	ILE	1648	15.470	14.047	-0.127	1.00 65.02
MOTA	1254	0	ILE	1648	16.633	14.245	0.233	1.00 66.85
ATOM	1255	N	HIS	1649	14.844	14.839	-0.995	1.00 65.85
MOTA	1256	CA	HIS	1649	15.505	15.992	-1.589	1.00 66.73
MOTA	1257	CB	HIS	1649	14.859	16.358	-2.934	1.00 65.67
ATOM	1258	CG	HIS	1649	15.142	15.388	-4.038	1.00 66.47
ATOM	1259	CD2	HIS	1649	16.253	14.686	-4.355	1.00 67.11
ATOM	1260	ND1	HIS	1649	14.210	15.064	-4.999	1.00 65.21
ATOM	1261	CEl	HIS	1649	14.733	14.216	-5.867	1.00 66.52
MOTA	1262	NE2	HIS	1649	15.974	13.966	-5.494	1.00 66.25
MOTA	1263	С	HIS	1649	15.505	17.200	-0.663	1.00 68.55
MOTA	1264	0	HIS	1649	15.636	18.341	-1.116	1.00 69.35
ATOM	1265	N	HIS	1650	15.273	16.963	0.629	1.00 71.25
ATOM	1266	CA	HIS	1650	15.262	18.026	1.633	1.00 73.53
ATOM	1267	CB	HIS	1650	13.849	18.551	1.860	1.00 76.79
MOTA	1268	CG	HIS	1650	13.342	19.448	0.765	1.00 83.36
ATOM	1269		HIS	1650	13.509	20.772	0.537	1.00 86.47
ATOM	1270		HIS	1650	12.571	18.984	-0.270	1.00 87.02
ATOM	1271		HIS	1650	12.279	19.983	-1.076	1.00 88.66
ATOM	1272		HIS	1650	12.840	21.080	-0.609	1.00 88.34
ATOM .	1273	С	HIS	1650	15.872	17.580	2.965	1.00 73.11
ATOM	1274	0	HIS	1650	15.686	18.241	3.977	1.00 73.23
ATOM	1275	N	ILE	1651	16.599	16.464	2.949	1.00 72.64
ATOM	1276	CA	ILE	1651	17.234	15.937	4.143	1.00 72.54
ATOM	1277	CB	ILE	1651	17.660	14.472	3.942	1.00 74.59
ATOM	1278	CG2	ILE	1651	18.463	13.966	5.142	1.00 75.52
ATOM	1279	CG1	ILE	1651	16.426	13.591	3.752	1.00 77.59
ATOM	1280		ILE	1651	16.747	12.141	3.472	1.00 80.12
ATOM	1281	C	ILE	1651	18.463	16.769	4.523	1.00 71.47
ATOM ATOM	1282	0	ILE	1651	19.326	17.022	3.688	1.00 72.40
ATOM	1283	N	ASP	1652	18.529	17.197	5.784	1.00 70.34
	1284	CA	ASP	1652	19.678	17.976	6.235	1.00 68.57
ATOM	1285	CB	ASP	1652	19.272	18.878	7.411	1.00 72.80
ATOM	1286	CG	ASP	1652	20.456	19.640	7.982	1.00 76.90
MOTA	1287	OD1		1652	21.463	19.888	7.287	1.00 79.62
MOTA	1288	OD2		1652	20.369	20.030	9.170	1.00 80.36
ATOM	1289	C	ASP	1652	20.771	17.007	6.652	1.00 66.01
ATOM	1290	0	ASP	1652	20.709	16.421	7.735	1.00 64.75
ATOM	1291	N	TYR	1653	21.778	16.868	5.808	1.00 64.05
ATOM	1292	CA	TYR	1653	22.906	15.978	6.074	1.00 63.55
ATOM	1293	CB	TYR	1653	23.829	15.913	4.855	1.00 63.81
ATOM	1294	CG	TYR	1653	23.316	14.993	3.771	1.00 65.65

ATOM	1295	CD1	TYR	1653	24.082	14.710	2.643	1.00 65.32
MOTA	1296	CE1	TYR	1653	23.638	13.810	1.674	1.00 68.40
ATOM	1297	CD2	TYR	1653	22.079	14.357	3.903	1.00 66.72
ATOM	1298	CE2	TYR	1653	21.626	13.451	2.940	1.00 69.93
ATOM	1299	CZ	TYR	1653	22.409	13.182	1.833	1.00 70.13
MOTA	1300	OH	TYR	1653	21.966	12.272	0.902	1.00 72.73
ATOM	1301	С	TYR	1653	23.708	16.334	7.328	1.00 62.96
ATOM	1302	0	TYR	1653	24.342	15.473	7.938	1.00 63.31
ATOM	1303	N	TYR	1654	23.653	17.598	7.727	1.00 63.02
MOTA	1304	CA	TYR	1654	24.379	18.065	8.902	1.00 63.89
MOTA	1305	CB	TYR	1654	24.896	19.491	8.684	1.00 60.37
ATOM	1306	CG	TYR	1654	26.012	19.565	7.669	1.00 59.33
ATOM	1307	CD1		1654	25.735	19.673	6.313	1.00 59.29
ATOM	1308	CE1		1654	26.759	19.687	5.362	1.00 61.50
ATOM	1309	CD2		1654	27.349	19.480	8.061	1.00 60.05
ATOM	1310	CE2	TYR	1654	28.384	19.498	7.119	1.00 61.35
ATOM	1311	CZ	TYR	1654	28.082	19.598	5.773	1.00 62.41
ATOM	1312	ОН	TYR	1654	29.098	19.589	4.842	1.00 60.57
MOTA	1313	С	TYR	1654	23.586	17.984	10.192	1.00 65.65
ATOM	1314	0	TYR	1654	24.104	18.321	11.252	1.00 67.31
ATOM	1315	N	LYS	1655	22.349	17.504	10.118	1.00 67.52
ATOM	1316	CA	LYS	1655	21.499	17.390	11.303	1.00 69.54
ATOM	1317	CB	LYS	1655	20.028	17.445	10.893	1.00 71.09
ATOM ATOM	1318	CG	LYS	1655	19.057	17.518	12.049	1.00 73.08
ATOM	1319	CD	LYS	1655	17.648	17.713	11.531	1.00 76.73
ATOM	1320 1321	CE NZ	LYS	1655	16.624	17.320	12.568	1.00 81.94
ATOM	1322	C	LYS	1655	15.232	17.521	12.072	1.00 84.53
ATOM	1323	0	LYS LYS	1655	21.783	16.102	12.076	1.00 70.33
ATOM	1324	N	LYS	1655 1656	21.952	15.032	11.478	1.00 70.43
ATOM	1325	CA	LYS	1656	21.825 22.093	16.218	13.403	1.00 70.11
ATOM	1326	СВ	LYS	1656	23.049	15.079 15.481	14.274 15.394	1.00 70.03
ATOM	1327	CG	LYS	1656	24.473	15.716	14.947	1.00 67.72 1.00 66.34
MOTA	1328	CD	LYS	1656	25.326	16.124	16.136	1.00 66.60
ATOM	1329	CE	LYS	1656	26.801	15.839	15.905	1.00 64.71
ATOM	1330	NZ	LYS	1656	27.612	16.059	17.138	1.00 62.71
ATOM	1331	С	LYS	1656	20.823	14.480	14.881	1.00 70.67
ATOM	1332	0	LYS	1656	19.759	15.104	14.864	1.00 70.87
MOTA	1333	N	THR	1657	20.941	13.265	15.412	1.00 69.38
ATOM	1334	CA	THR	1657	19.818	12.586	16.035	1.00 68.30
MOTA	1335	CB	THR	1657	20.052	11.051	16.101	1.00 69.30
MOTA	1336	OG1	THR	1657	21.179	10.757	16.941	1.00 68.20
ATOM	1337	CG2	THR	1657	20.310	10.479	14.713	1.00 69.71
MOTA	1338	С	THR	1657	19.706	13.145	17.445	1.00 67.60
ATOM	1339	0	THR	1657	20.521	13.971	17.846	1.00 67.40
MOTA	1340	N·	ALA	1658	18.715	12.694	18.206	1.00 67.83
ATOM	1341	CA	ALA	1658	18.564	13.163	19.582	1.00 67.73
ATOM	1342	CB	ALA	1658	17.345	12.503	20.234	1.00 68.87
ATOM	1343	С	ALA	1658	19.833	12.820	20.364	1.00 66.59
MOTA	1344	0	ALA	1658	20.368	13.640	21.115	1.00 66.33
MOTA	1345	N	asn	1659	20.343	11.616	20.129	1.00 65.38
ATOM	1346	CA	ASN	1659	21.545	11.143	20.801	1.00 62.65

ATOM	1347	CB	ASN	1659	21.702	9.638	20.616	1.00	63.61
MOTA	1348	CG	ASN	1659	22.548	9.009	21.697	1.00	64.09
MOTA	1349	OD1	ASN	1659	22.526	9.451	22.850	1.00	63.69
ATOM	1350	ND2	ASN	1659	23.279	7.959	21.345	1.00	64.10
MOTA	1351	C	ASN	1659	22.808	11.844	20.321	1.00	60.46
ATOM	1352	0	ASN	1659	23.882	11.601	20.856	1.00	60.78
ATOM	1353	N	GLY	1660	22.671	12.675	19.285	1.00	58.84
ATOM	1354	CA	GLY	1660	23.803	13.407	18.735	1.00	56.69
ATOM	1355	С	GLY	1660	24.570	12.721	17.616	1.00	56.40
ATOM	1356	0	GLY	1660	25.738	13.028	17.377	1.00	56.43
ATOM	1357	N	ARG	1661	23.929	11.779	16.937	1.00	56.00
MOTA	1358	CA	ARG	1661	24.585	11.048	15.849	1.00	53.80
ATOM	1359	CB	ARG	1661	24.312	9.540	15.952	1.00	54.52
MOTA	1360	CG	ARG	1661	24.876	8.879	17.218	1.00	55.28
ATOM	1361	CD	ARG	1661	24.556	7.395	17.226	1.00	58.01
ATOM	1362	NE	ARG	1661	25.051	6.670	18.396	1.00	58.41
ATOM	1363	\mathbf{cz}	ARG	1661	24.91B	5.355	18.559	1.00	59.08
ATOM	1364	NH1	ARG	1661	24.306	4.637	17.623	1.00	55.82
ATOM	1365	NH2	ARG	1661	25.394	4.762	19.652	1.00	57.53
MOTA	1366	C	ARG	1661	24.139	11.581	14.491	1.00	51.03
MOTA	1367	0	ARG	1661	23.160	12.323	14.401	1.00	48.69
ATOM	1368	N	LEU	1662	24.859	11.189	13.440	1.00	48.33
ATOM	1369	CA	LEU	1662	24.565	11.647	12.087	1.00	45.87
ATOM	1370	CB	LEU	1662	25.839	12.199	11.426	1.00	46.18
ATOM	1371	ÇG	LEU	1662	26.374	13.511	12.016	1.00	45.78
ATOM	1372	CD1	LEU	1662	27.856	13.681	11.722	1.00	45.92
MOTA	1373	CD2	LEU	1662	25.576	14.698	11.489	1.00	44.92
ATOM	1374	C	LEU	1662	23.961	10.542	11.230	1.00	43.02
MOTA	1375	0	LEU	1662	24.647	9.607	10.811	1.00	42.04
ATOM	1376	N	PRO	1663	22.648	10.640	10.968	1.00	41.48
ATOM	1377	CD	PRO	1663	21.769	11.718	11.468		40.54
MOTA	1378	CA	PRO	1663	21.886	9.680	10.161		39.60
ATOM	1379	CB	PRO	1663	20.582	10.424	9.889		38.77
ATOM	1380	CG	PRO	1663	20.386	11.183	11.151		40.83
ATOM	1381	C	PRO	1663	22.578	9.273	8.860		35.90
MOTA	1382	0	PRO	1663	22.448	8.124	8.427		36.85
MOTA	1383	N	VAL	1664	23.356	10.180	8.276		33.16
MOTA	1384	CA	VAL	1664	24.053		7.024		32.51
ATOM	1385	CB	VAL	1664	24.851	11.106	6.439		32.44
ATOM	1386		VAL	1664	23.917	12.213	6.065		26.99
ATOM	1387		VAL	1664	25.897	11.607	7.421		29.84
ATOM	1388	C	VAL	1664	24.989	8.675	7.158		30.30
ATOM	1389	0 N	VAL	1664	25.400	8.091	6.161		30.16
ATOM	1390	N	LYS	1665	25.278	8.276	8.393		27.72
MOTA	1391	CA	LYS	1665	26.170	7.151	8.649		27.96
ATOM	1392	CB	LYS	1665	26.808	7.276	10.025		26.42
ATOM	1393	CG	LYS	1665	27.857	8.351	10.061		28.20
ATOM	1394		LYS	1665	28.221	8.754	11.478		32.47
ATOM	1395	CE	LYS	1665	29.398	9.720	11.468		32.33
ATOM	1396	NZ	LYS	1665	29.713	10.231	12.819		30.38
ATOM	1397	С	LYS	1665	25.522	5.794	8.486		25.81
ATOM	1398	0	LYS	1665	26.159	4.769	8.691	1.00	27.53

MOTA	1399	N	TRP	1666	24.247	5.793	8.120	1.00 26.13
MOTA	1400	CA	TRP	1666	23.499	4.554	7.896	1.00 25.88
ATOM	1401	CB	TRP	1666	22.259	4.537	8.800	1.00 26.15
ATOM	1402	CG	TRP	1666	22.547	4.067	10.226	1.00 28.12
MOTA	1403	CD2	TRP	1666	23.020	4.864	11.324	1.00 26.14
MOTA	1404	CE2	TRP	1666	23.154	4.009	12.438	1.00 24.97
MOTA	1405	CE3	TRP	1666	23.349	6.225	11.475	1.00 25.14
MOTA	1406	CD1	TRP	1666	22.408	2.795	10.715	1.00 26.09
MOTA	1407	NE1	TRP	1666	22.777	2.751	12.034	1.00 22.55
MOTA	1408	CZ2	TRP	1666	23.606	4.453	13.684	1.00 25.32
ATOM	1409	CZ3	TRP	1666	23.795	6.664	12.712	1.00 21.72
ATOM	1410	CH2	TRP	1666	23.920	5.782	13.798	1.00 23.77
MOTA	1411	C:	TRP	1666	23.092	4.444	6.425	1.00 24.79
MOTA	1412	0	TRP	1666	22.662	3.390	5.971	1.00 25.26
ATOM	1413	N	MET	1667	23.350	5.508	5.664	1.00 24.21
MOTA	1414	CA	MET	1667	22.963	5.568	4.252	1.00 23.79
MOTA	1415	CB	MET	1667	22.796	7.018	3.809	1.00 25.08
ATOM	1416	CG	MET	1667	21.793	7.813	4.564	1.00 32.58
ATOM	1417	SD	MET	1667	21.778	9.495	3.910	1.00 41.43
ATOM	1418	CE	MET	1667	21.011	9.209	2.387	1.00 40.85
ATOM	1419	C	MET	1667	23.938	4.942	3.279	1.00 22.52
ATOM	1420	0	MET	1667	25.139	5.173	3.362	1.00 23.63
MOTA	1421	N	ALA	1668	23.406	4.195	2.324	1.00 22.77
MOTA	1422	CA	ALA	1668	24.218	3.576.	1.278	1.00 24.91
ATOM	1423	CB	ALA	1668	23.342	2.672	0.396	1.00 24.41
MOTA	1424	C	ALA	1668	24.800	4.706	0.438	1.00 26.66
MOTA	1425	0	ALA	1668	24.163	5.748	0.251	1.00 24.54
MOTA	1426	N	PRO	1669	26.011	4.511	-0.101	1.00 26.97
ATOM	1427	CD	PRO	1669	26.935	3.374	0.066	1.00 26.23
ATOM	1428	CA	PRO	1669	26.614	5.563	-0.919	1.00 26.05
ATOM	1429	CB	PRO	1669	27.855	4.876	-1.482	1.00 24.03
MOTA	1430	CG	PRO	1669	28.259	3.946	-0.358	1.00 26.27
ATOM	1431	C	PRO	1669	25.687	6.048	-2.030	1.00 26.44
MOTA	1432	0	PRO	1669	25.576	7.250	-2.263	1.00 27.72
ATOM	1433	N	GLU	1670	24.971	5.137	-2.685	1.00 27.16
ATOM	1434	CA	GLU	1670	24.093	5.553	-3.769	1.00 27.63
ATOM	1435	CB	GLU	1670	23.613	4.365	-4.614	1.00 29.35
MOTA	1436	CG	GLU	1670	22.545	3.492	-3.980	1.00 29.16
ATOM	1437	CD	GLU	1670	23.089	2.238	-3.310	1.00 28.03
MOTA	1438	OE1	GLU	1670	22.248	1.430	-2.874	1.00 24.12
ATOM	1439	OE2	GLU	1670	24.325	2.040	-3.215	1.00 26.07
MOTA	1440	С	GLU	1670	22.931	6.407	-3.301	1.00 25.52
ATOM	1441	0	GLU	1670	22.477	7.281	-4.042	1.00 24.12
ATOM	1442	N	ALA	1671	22.452	6.163	-2.084	1.00 27.74
ATOM	1443	CA	ALA	1671	21.337	6.928	-1.510	1.00 27.65
ATOM	1444	CB	ALA	1671	20.729	6.189	-0.319	1.00 23.18
ATOM	1445	С	ALA	1671	21.860	8.283	-1.065	1.00 28.22
ATOM	1446	0	ALA	1671	21.234	9.310	-1.305	1.00 28.51
ATOM	1447	N	LEU	1672	23.011	8.266	-0.406	1.00 30.60
ATOM	1448	CA	LEU	1672	23.647	9.484	0.074	1.00 32.67
ATOM	1449	CB	LEU	1672	24.831	9.127	0.952	1.00 32.05
MOTA	1450	CG	LEU	1672	25.662	10.264	1.527	1.00 34.00

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MOTA	1451	CD	LEU	1672	24.874	10.981	2.577	1.00 38.85
MOTA	1452		LEU	1672	26.910	9.667	2.149	1.00 35.22
MOTA	1453	. C	LEU	1672	24.121	10.398	-1.067	1.00 37.10
ATOM	1454	0	LEU	1672	23.799	11.580	-1.086	1.00 37.19
MOTA	1455	N	PHE	1673	24.905	9.858	-1.997	1.00 37.60
ATOM	1456	CA	PHE	1673	25.403	10.664	-3.102	1.00 37.11
ATOM	1457	CB	PHE	1673	26.692	10.061	-3.667	1.00 35.24
ATOM	1458	CG	PHE	1673	27.782	9.857	-2.644	1.00 33.54
MOTA	1459	CD1	PHE	1673	28.456	8.633	-2.566	1.00 31.54
MOTA	1460	CD2	PHE	1673	28.143	10.874	-1.762	1.00 33.10
MOTA	1461	CE1	PHE	1673	29.467	8.421	-1.623	1.00 34.66
ATOM	1462	CE2	PHE	1673	29.156	10.678	-0.816	1.00 35:41
MOTA	1463	CZ.	PHE	-1673	29.819	9.444	-0.748	1.00 34.81
ATOM	1464	C	PHE	1673	24.406	10.890	-4.245	1.00 39.03
ATOM	1465	0	PHE	1673	24.276	11.997	-4.734	1.00 39.02
ATOM	1466	N	ASP	1674	23.693	9.844	-4.651	1.00 42.35
MOTA	1467	CA	ASP	1674	22.757	9.931	-5.762	1.00 41.59
MOTA	1468	CB	ASP	1674	22.957	8.736	-6.700	1.00 46.08
ATOM	1469	CG	ASP	1674	24.384	8.617	-7.201	1.00 51.20
ATOM	1470	OD1	ASP	1674	25.057	9.663	-7.333	1.00 53.97
MOTA	1471	OD2	ASP	1674	24.822	7.470	-7.469	1.00 50.65
ATOM	1472	C	ASP	1674	21.263	9.999	-5.418	1.00 42.89
ATOM	1473	0	ASP	1674	20.427	10.079	-6.317	1.00 41.95
ATOM	1474	N	ARG	1675	20.923	9.899	-4.134	1.00 42.82
ATOM	1475	CA	ARG	1675	19.521	9.944	-3.706	1.00 42.64
MOTA	1476	CB	ARG	1675	18.890	11.300	-4.028	1.00 48.80
ATOM	1477	CG	ARG	1675	19.480	12.449	-3.252	1.00 61.19
ATOM	1478	CD	ARG	1675	19.407	13.727	-4.068	1.00 72.90
MOTA	1479	NE	ARG	1675	20.025	14.854	-3.381	1.00 83.15
MOTA	1480	CZ	ARG	1675	19.652	16.123	-3.539	1.00 88.21
ATOM	1481	NH1	ARG	1675	18.662	16.439	-4.365	1.00 89.58
ATOM	1482	NH2	ARG	1675	20.265	17.085	-2.860	1.00 92.07
ATOM	1483	C	ARG	1675	18.674	8.825	-4.299	1.00 38.05
MOTA	1484	0	ARG	1675	17.495	9.005	-4.588	1.00 38.87
ATOM	1485	N	ILE	1676	19.281	7.658	-4.479	1.00 34.44
ATOM	1486	CA	ILE	1676	18.576	6.514	-5.012	1.00 30.11
ATOM	1487	CB	ILE	1676	19.378	5.825	-6.096	1.00 29.58
ATOM	1488	CG2	ILE	1676	18.509	4.850	-6.797	1.00 30.72
ATOM	1489		ILE	1676	19.835	6.868	-7.116	1.00 34.29
ATOM	1490	CD1	ILE	1676	20.798	6.348	-8.145	1.00 41.15
ATOM	1491	С	ILE	1676	18.315	5.541	-3.874	1.00 26.90
ATOM	1492	0	ILE	1676	19.236	4.898	-3.364	1.00 22.06
ATOM	1493	N	TYR	1677	17.056	5.465	-3.454	1.00 28.17
ATOM	1494	CA	TYR	1677	16.677	4.589	-2.350	1.00 26.80
MOTA	1495	CB	TYR	1677	15.742	5.310	-1.398	1.00 26.05
ATOM	1496	CG	TYR	1677	16.442	6.367	-0.580	1.00 26.92
ATOM	1497		TYR	1677	16.510	7.693	-1.018	1.00 23.98
ATOM	1498	CE1		1677	17.129	8.665	-0.250	1.00 23.90
ATOM	1499	CD2		1677	17.022	6.048	0.644	1.00 26.99
ATOM	1500		TYR	1677	17.642	7.017	1.414	1.00 24.87
ATOM	1501		TYR	1677	17.685	8.315	0.968	1.00 26.44
ATOM	1502	OH	TYR	1677	18.227	9.273	1.783	1.00 30.89

MOTA	1503	С	TYR	1677	16.006	3.350	-2.894	1.00 26.30
MOTA	1504	0	TYR	1677	15.080	3.445	-3.703	1.00 28.12
MOTA	1505	N	THR	1678	16.489	2.197	-2.458	1.00 25.46
ATOM	1506	CA	THR	1678	15.973	0.918	-2.927	1.00 26.27
MOTA	1507	CB	THR	1678	16.904	0.336	-3.994	1.00 28.43
ATOM	1508	OG1	THR	1678	18.185	0.095	-3.405	1.00 30.59
ATOM	1509	CG2	THR	1678	17.068	1.305	-5.174	1.00 26.56
MOTA	1510	С	THR	1678	15.987	-0.049	-1.758	1.00 24.60
MOTA	1511	0	THR	1678	16.476	0.277	-0.693	1.00 27.15
ATOM	1512	N	HIS	1679	15.500	-1.260	-1.974	1.00 23.23
ATOM	1513	CA	HIS	1679	15.496	-2.276	-0.933	1.00 21.51
MOTA	1514	CB	HIS	1679	14.747	-3.520	-1.411	1.00 20.84
ATOM	1515	CG	HIS -	1679	13.297	-3.279	-1.695	1.00 21.48
MOTA	1516	CD2	HIS	1679	12.552	-3.476	-2.812	1.00 22.71
ATOM	1517	ND1	HIS	1679	12.423	-2.795	-0.741	1.00 27.21
MOTA	1518	CE1	HIS	1679	11.206	-2.713	-1.255	1.00 22.60
MOTA	1519	NE2	HIS	1679	11.255	-3.116	-2.515	1.00 23.66
MOTA	1520	С	HIS	1679	16.976	-2.591	-0.665	1.00 20.81
ATOM	1521	0	HIS	1679	17.358	-2.954	0.451	1.00 22.50
MOTA	1522	Ν.	GLN	1680	17.799	-2.382	-1.695	1.00 19.58
MOTA	1523	CA	GLN	1680	19.248	-2.587	-1.657	1.00 20.89
ATOM	1524	CB	GLN	1680	19.860	-2.400	-3.038	1.00 23.76
ATOM	1525	CG	GLN	1680	19.896	-3.651	-3.877	1.00 34.08
ATOM	1526	ന	GLN	1680	19.015	-3.559	-5.096	1.00 37.77
ATOM	1527	OE1	GLN	1680	18.069	-2.780	-5.122	1.00 43.23
ATOM	1528	NE2	GLN	1680	19.321	-4.356	-6.113	1.00 37.02
ATOM	1529	C	GLN	1680	19.913	-1.609	-0.724	1.00 20.72
MOTA	1530	0	GLN	1680	20.814	-1.981	0.021	1.00 21.53
MOTA	1531	N	SER	1681	19.514	-0.350	-0.773	1.00 21.01
ATOM	1532	CA	SER	1681	20.128	0.606	0.135	1.00 23.86
MOTA	1533	CB	SER	1681	19.841	2.065	-0.248	1.00 21.10
MOTA	1534	OG	SER	1681	18.473	2.290	-0.506	1.00 23.18
MOTA	1535	C	SER	1681	19.695	0.292	1.564	1.00 23.91
MOTA	1536	0	SER	1681	20.457	0.542	2.495	1.00 26.70
ATOM	1537	N	ASP	1682	18.511	-0.303	1.739	1.00 21.71
ATOM	1538	CA	ASP	1682	18.044	-0.662	3.080	1.00 21.28
ATOM	1539	CB	ASP	1682	16.595	-1.149	3.070	1.00 23.22
MOTA	1540	CG	ASP	1682	15.569	-0.016	3.198	1.00 23.08
MOTA	1541	OD1		1682	14.363	-0.282	3.017	1.00 21.99
MOTA	1542	OD2		1682	15.948	1.135	3.498	1.00 24.42
ATOM	1543	С	ASP	1682	18.955	-1.756	3.611	1.00 20.86
ATOM	1544	0	ASP	1682	19.289	-1.770	4.799	1.00 21.62
MOTA	1545	N	VAL	1683	19.398	-2.649	2.727	1.00 21.60
ATOM	1546	CA	VAL	1683	20.307	-3.732	3.122	1.00 22.27
MOTA	1547	CB	VAL	1683	20.515	-4.740	1.965	1.00 22.22
ATOM	1548	CG1		1683	21.587	-5.777	2.315	1.00 21.52
MOTA	1549	CG2		1683	19.187	-5.437	1.662	1.00 20.89
ATOM	1550	С	VAL	1683	21.618	-3.150	3.666	1.00 21.96
MOTA	1551	0	VAL	1683	22.107	-3.577	4.705	1.00 24.39
ATOM	1552	N	TRP	1684	22.172	-2.160	2.970	1.00 22.01
MOTA	1553	CA	TRP	1684	23.375	-1.489	3.449	1.00 23.06
MOTA	1554	CB	TRP	1684	23.685	-0.273	2.566	1.00 20.25

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MOTA 1555 24.808 3.069 CG TRP 1684 0.549 1.00 22.35 MOTA 1556 CD2 TRP 1684 2.503 26.118 0.644 1.00 24.14 **ATOM** 1557 CE2 TRP 1684 26.879 1.500 3.334 1.00 23.68 **ATOM** 1558 CE3 TRP 1684 26.728 0.091 1.370 1.00 25.09 **ATOM** 1559 CD1 TRP 1684 24.825 1.346 4.193 1.00 22.52 MOTA 1560 NE1 TRP 1684 26.066 1.915 4.355 1.00 21.48 **ATOM** 1561 CZ2 TRP 1684 28.216 1.815 3.061 1.00 20.56 **ATOM** 1562 CZ3 TRP 1684 28.059 0.405 1.095 1.00 23.92 MOTA 1563 CH2 TRP 1684 28.785 1.257 1.942 1.00 23.18 MOTA 1564 C TRP 1684 23.105 -1.025 4.903 1.00 23.96 -1.308 ATOM 1565 0 TRP 1684 23.889 5.815 1.00 25.98 MOTA 1566 N SER 21.992 1685 -0.332 5.118 1.00 24.68 -- ATOM CA SER 1685 1567 21.615 0.144 6.447 -1.00 22.75 **ATOM** 1568 CB SER 1685 20.266 0.870 6.376 1.00 21.11 MOTA 1569 OG SER 1685 20.276 1.950 5.452 1.00 21.98 **ATOM** 1570 C SER 1685 21.516 -1.011 7.457 1.00 23.06 ATOM 1571 0 SER 1685 21.865 -0.850 8.638 1.00 22.55 MOTA 1572 N PHE 1686 21.041 -2.168 6.998 1.00 21.83 ATOM 1573 CA PHE 1686 20.915 -3.340 7.854 1.00 21.92 1574 MOTA CB PHE 1686 20.153 -4.457 7.129 1.00 18.02 MOTA 1575 CG PHE 1686 19.965 -5.683 7.971 1.00 20.86 **ATOM** 1576 CD1 PHE 1686 19.142 -5.641 9.108 1.00 18.76 **ATOM** 1577 CD2 PHE 1686 20.669 -6.853 7.688 1.00 18.96 MOTA 1578 CE1 PHE 1686 19.023 -6.743 9.947 1.00 19.29 **ATOM** 1579 CE2 PHE 1686 20.554 -7.965 8.514 1.00 19.27 MOTA 1580 CZ PHE 1686 19.732 -7.908 9.653 1.00 21.91 **ATOM** 1581 C PHE 1686 22.304 -3.845 8.316 1.00 22.11 MOTA 1582 O PHE 1686 22.473 -4.378 9.436 1.00 21.35 ATOM 1583 N GLY 1687 23.294 -3.691 7.436 1.00 20.48 MOTA CA GLY 1584 1687 24.653 -4.079 7.769 1.00 20.41 **ATOM** C 1585 GLY 1687 25.185 -3.211 8.899 1.00 19.03 MOTA 1586 0 GLY 1687 25.857 -3.714 9.808 1.00 20.27 MOTA 1587 N VAL 1688 24.893 -1.906 8.829 1.00 20.57 MOTA 1588 CA VAL 1688 25.296 -0.937 1.00 21.14 9.860 MOTA 1589 CB VAL 1688 24.974 0.548 9.467 1.00 20.78 MOTA 1590 CG1 VAL 1688 25.440 1.493 10.564 1.00 21.51 MOTA 1591 VAL CG2 1688 25.681 0.923 8.186 1.00 19.70 **ATOM** 1592 C VAL 1688 24.547 -1.297 11.142 1.00 23.16 MOTA 1593 O VAL 1688 25.126 -1.271 12.225 1.00 24.14 MOTA 1594 LEU 1689 N 23.264 -1.648 11.021 1.00 24.50 MOTA 1595 CA LEU 1689 22.465 -2.058 12.187 1.00 25.93 MOTA 1596 CB LEU 1689 21.008 -2.316 11.776 1.00 25.42 **MOTA** 1597 CG LEU 1689 19.933 -2.392 12.874 1.00 26.29 **ATOM** 1598 CD1 LEU 1689 18.572 -2.053 12.272 1.00 23.43 MOTA 1599 CD2 LEU 19.885 1689 -3.768 13.543 1.00 25.66 MOTA 1600 LEU · C 1689 23.080 -3.330 12.797 1.00 28.01 **ATOM** 1601 0 LEU 1689 23.203 -3.426 14.016 1.00 30.06 **ATOM** 1602 N LEU 1690 23.487 -4.287 11.956 1.00 27.19 MOTA 1603 CA LEU 1690 24.111 -5.520 12.457 1.00 25.29 1690 **ATOM** 1604 CB LEU 24.556 -6.446 11.315 1.00 24.98 **ATOM** 1605 CG LEU 1690 23.594 -7.390 10.589 1.00 24.85 MOTA 1606 CD1 LEU 1690 24.385 -8.132 9.538 1.00 24.22

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ATOM	1607	CD2	LEU	1690	22.960	-8.434	11.512	1.00 19.10
MOTA	1608	C	LEU	1690	25.326	-5.123	13.291	1.00 24.70
ATOM	1609	0	LEU	1690	25.521	-5.624	14.408	1.00 23.57
MOTA	1610	N	TRP	1691	26.117	-4.197	12.747	1.00 23.68
ATOM	1611	CA	TRP	1691	27.316	-3.693	13.425	1.00 24.83
ATOM	1612	CB	TRP	1691	27.998	-2.621	12.567	1.00 20.94
ATOM	1613	CG	TRP	1691	29.331	-2.173	13.105	1.00 24.80
MOTA	1614	CD2	TRP	1691	29.565	-1.082	14.004	1.00 23.71
MOTA	1615	CE2	TRP	1691	30.966	-0.996	14.208	1.00 23.81
ATOM	1616	CE3	TRP	1691	28.726	-0.167	14.652	1.00 22.20
MOTA	1617	CD1	TRP	1691	30.570	-2.702	12.811	1.00 24.44
MOTA	1618	NE1	TRP	1691	31.550	-1.995	13.471	1.00 25.38
ATOM -	1619	CZ2	TRP	1691	31.543	-0.022	15.034	1.00 24.39
MOTA	1620	CZ3	TRP	1691	29.300	0.799	15.484	1.00 21.99
ATOM	1621	CH2	TRP	1691	30.700	0.862	15.665	1.00 25.57
MOTA	1622	C	TRP	1691	26.998	-3.131	14.823	1.00 25.87
ATOM	1623	0	TRP	1691	27.772	-3.301	15.750	1.00 27.39
MOTA	1624	N	GLU	1692	25.865	-2.448	14.956	1.00 26.45
ATOM	1625	CA	GLU	1692	25.452	-1.869	16.238	1.00 25.13
MOTA	1626	CB	GLU	1692	24.257	-0.933	16.068	1.00 23.56
ATOM	1627	CG	GLU	1692	24.365	0.091	14.962	1.00 18.73
ATOM	1628	CD	GLU	1692	23.111	0.935	14.880	1.00 23.79
ATOM	1629	OE1	GLU	1692	22.303	0.722	13.962	1.00 22.70
MOTA	1630	OE2	GLU	1692	22.919	1.819	15.738	1.00 25.63
ATOM	1631	C	GLU	1692	25.072	-2.963	17.225	1.00 25.28
ATOM	1632	0	GLU	1692	25.278	-2.818	18.422	1.00 27.65
MOTA	1633	N	ILE	1693	24.484	-4.046	16.720	1.00 26.23
ATOM	1634	CA	ILE	1693	24.080	-5.164	17.565	1.00 23.81
MOTA	1635	CB	ILE	1693	23.177	-6.203	16.787	1.00 22.99
MOTA	1636	CG2	ILE	1693	22.966	-7.465	17.637	1.00 21.67
MOTA	1637	CG1	ILE	1693	21.820	-5.569	16.416	1.00 20.23
ATOM	1638	CD1	ILE	1693	20.964	-6.395	15.435	1.00 13.67
ATOM	1639	С	ILE	1693	25.322	-5.843	18.133	1.00 24.77
ATOM	1640	0	ILE	1693	25.401	-6.126	19.324	1.00 24.94
ATOM	1641	N	PHE	1694	26.329	-6.051	17.304	1.00 27.59
ATOM	1642	CA	PHE	1694	27.503	-6.709	17.827	1.00 29.42
ATOM	1643	CB	PHE	1694	28.122	-7.623	16.771	1.00 29.37
ATOM	1644	CG	PHE	1694	27.142	-B.649	16.263	1.00 27.99
ATOM	1645	CDI		1694	26.522	-8.486	15.034	1.00 28.43
ATOM	1646	CD2		1694	26.751	-9.709	17.074	1.00 27.86
ATOM	1647	CE1		1694	25.525	-9.355	14.625	1.00 30.12
ATOM	1648	CE2		1694		-10.586	16.674	1.00 25.78
ATOM	1649	CZ	PHE	1694	25.136	-10.408	15.453	1.00 26.17
ATOM	1650	С	PHE	1694	28.495	-5.821	18.578	1.00 29.83
ATOM	1651	0	PHE	1694	29.485	-6.305	19.126	1.00 32.81
MOTA	1652	N·	THR	1695	28.217	-4.516	18.635	1.00 28.35
MOTA	1653	CA	THR	1695	29.044	-3.598	19.419	1.00 25.39
MOTA	1654	CB	THR	1695	29.540	-2.379	18.627	1.00 21.81
ATOM	1655		THR	1695	28.422	-1.628	18.137	1.00 21.54
MOTA	1656		THR	1695	30.457	-2.816	17.508	1.00 16.93
MOTA	1657	С	THR	1695	28.198	-3.126	20.604	1.00 26.16
ATOM	1658	0	THR	1695	28.620	-2.268	21.386	1.00 26.77

ATOM	1659	N	LEU	1696	27.023	-3.747	20.747	1.00 26.87
ATOM	1660	CA	LEU	1696	26.069	-3.446	21.813	1.00 27.64
ATOM	1661	CB	LEU	1696	26.572	-3.977	23.156	1.00 30.54
ATOM	1662	CG	LEU	1696	26.903	-5.456	23.182	1.00 29.75
ATOM	1663	CD1	LEU	1696	27.448	-5.821	24.546	1.00 32.53
ATOM	1664	CD2	LEU	1696	25.658	-6.234	22.882	1.00 33.79
ATOM	1665	С	LEU	1696	25.727	-1.984	21.946	1.00 25.51
ATOM	1666	0	LEU	1696	25.824	-1.410	23.025	1.00 27.90
ATOM	1667	N	GLY	1697	25.265	-1.395	20.857	1.00 26.48
ATOM	1668	CA	GLY	1697	24.899	0.007	20.859	1.00 25.81
ATOM	1669	С	GLY	1697	26.040	0.900	20.452	1.00 26.40
ATOM	1670	0	GLY	1697	26.055	2.090	20.760	1.00 29.69
 - MOTA	1671	N	GLY	1698	27.008	0.330	19.748	1:00 27.65
MOTA	1672	CA	GLY	1698	28.150	1.110	19.314	1.00 28.38
MOTA	1673	С	GLY	1698	27.795	2.186	18.310	1.00 30.13
ATOM	1674	0	GLY	1698	26.896	2.028	17.496	1.00 32.55
ATOM	1675	N	SER	1699	28.520	3.295	18.375	1.00 30.56
MOTA	1676	CA	SER	1699	28.304	4.420	17.491	1.00 32.11
ATOM	1677	CB	SER	1699	28.622	5.714	18.246	1.00 33.58
ATOM	1678	OG	SER	1699	28.578	6.863	17.407	1.00 38.87
ATOM	1679	С	SER	1699	29.203	4.269	16.268	1.00 32.10
ATOM	1680	0	SER	1699	30.408	4.073	16.403	1.00 31.12
MOTA	1681	N	PRO	1700	28.629	4.324	15.062	1.00 32.70
MOTA	1682	CD	PRO	1700	27.204	4.482	14.745	1.00 34.35
MOTA	1683	CA	PRO	1700	29.427	4.192	13.837	1.00 32.25
MOTA	1684	CB	PRO	1700	28.358	4.096	12.736	1.00 32.85
MOTA	1685	CG	PRO	1700	27.101	3.713	13.461	1.00 35.54
ATOM	1686	С	PRO	1700	30.258	5.456	13.651	1.00 31.84
MOTA	1687	0	PRO	1700	29.792	6.550	13.983	1.00 31.56
ATOM	1688	N	TYR	1701	31.487	5.306	13.170	1.00 31.07
ATOM	1689	CA	TYR	1701	32.372	6.441	12.910	1.00 32.41
ATOM	1690	CB	TYR	1701	32.039	7.055	11.537	1.00 32.39
MOTA	1691	CG	TYR	1701	32.088	6.092	10.378	1.00 35.63
MOTA	1692	CD1		1701	30.936	5.807	9.638	1.00 37.94
MOTA	1693	CE1		1701	30.977	4.955	8.535	1.00 40.79
MOTA	1694	CD2		1701	33.293	5.495	9.990	1.00 37.49
ATOM	1695	CE2		1701	33.351	4.646	8.886	1.00 41.82
ATOM	1696	CZ	TYR	1701	32.190	4.382	8.160	1.00 45.96
MOTA	1697	OH	TYR	1701	32.251	3.572	7.039	1.00 55.61
ATOM	1698	C	TYR	1701	32.377	7.559	13.970	1.00 32.85
ATOM	1699	0	TYR	1701	32.066	8.711	13.679	1.00 32.41
ATOM	1700	N	PRO	1702	32.753	7.229	15.215	1.00 34.48
ATOM	1701		PRO	1702	33.288	5.946	15.695	1.00 35.64
ATOM	1702		PRO	1702	32.775	8.258	16.270	1.00 33.68
ATOM	1703		PRO	1702	33.321	7.499	17.482	1.00 32.52
ATOM	1704		PRO	1702	33.063	6.061	17.166	1.00 38.81
ATOM	1705		PRO	1702	33.736	9.388	15.919	1.00 33.47
MOTA	1706		PRO	1702	34.875	9.145	15.522	1.00 34.66
MOTA	1707		GLY	1703	33.275	10.625	16.089	1.00 35.31
MOTA	1708		GLY	1703	34.101	11.792	15.802	1.00 32.51
ATOM	1709		GLY	1703	34.232	12.166	14.339	1.00 33.68
ATOM	1710	0	GLY	1703	34.904	13.146	14.005	1.00 31.22

ATOM	1711	N	VAL	1704	33.583	11.404	13.462	1.00 35	.00			
ATOM	1712	CA	VAL	1704	33.641	11.658	12.026	1.00 33	.25			
ATOM	1713	CB	VAL	1704	33.679	10.335	11.241	1.00 31	.04			
ATOM	1714	CG1	VAL	1704	33.825	10.605	9.766	1.00 32	. 72			
ATOM	1715	CG2	VAL	1704	34.825	9.477	11.727	1.00 26	. 97			
ATOM	1716	C	VAL	1704	32.475	12.529	11.533	1.00 34	. 7 5		•	
ATOM	1717	0	VAL	1704	31.316	12.151	11.643	1.00 36	. 79			
MOTA	1718	N	PRO	1705	32.787	13.735	11.032	1.00 35	.01			
ATOM	1719	CD	PRO	1705	34.133	14.333	11.086	1.00 35	.61			
ATOM	1720	CA	PRO	1705	31.801	14.685	10.512	1.00 35	.33			
ATOM	1721	CB	PRO	1705	32.539	16.020	10.617	1.00 35	. 59			
ATOM	1722	CG	PRO	1705	33.950	15.625	10.339	1.00 37	.23			
ATOM	1723	G.	-PRO	1705	31.388	14.375	9.074	1.00 36	.33	:- '	 	
ATOM	1724	0	PRO	1705	32.125	13.695	8.355	1.00 38	.44			
MOTA	1725	N	VAL	1706	30.240	14.912	8.649	1.00 34	. 93			
ATOM	1726	CA	VAL	1706	29.675	14.704	7.303	1.00 35	.19			
ATOM	1727	CB	VAL	1706	28.607	15.791	6.984	1.00 36	.19			
ATOM	1728		VAL	1706	28.011	15.586	5.586	1.00 36	.30			
ATOM	1729		VAL	1706	27.494	15.7 39	8.028	1.00 32	. 74			
ATOM	1730	C	VAL	1706	30.696	14.632	6.155	1.00 36	. 20			
ATOM	1731	0	VAL	1706	30.796	13.618	5.463	1.00 38	. 16			
ATOM	1732	N	GLU	1707	31.479	15.695	6.020	1.00 34	. 38			
ATOM	1733	CA	GLU	1707	32.500	15.819	4.987	1.00 33	. 75			•
ATOM	1734	СВ	GLU	1707	33.181	17.184	5.083	1.00 35	.79			
ATOM	1735	C	GLU	1707	33.567	14.731	4.982	1.00 31				
ATOM	1736	0	GLU	1707	34.036	14.311	3.923	1.00 32				
ATOM	1737	N	GLU	1708	33.964	14.280	6.160	1.00 29				
ATOM	1738	CA	GLU	1708	34.987	13.249	6.249	1.00 31				
ATOM	1739	CB	GLU	1708	35.567	13.204	7.664	1.00 36				
ATOM ATOM	1740	CG	GLU	1708	36.189	14.508	8.144	1.00 44				
ATOM	1741	CD	GLU	1708	37.444	14.923	7.383	1.00 55				
ATOM	1742 1743	OE1		1708	38.059	14.082	6.681	1.00 61				
ATOM	1744	OE2 C	GLU	1708	37.830	16.115	7.517	1.00 60				
ATOM	1745	0	GLU	1708 1708	34.365	11.906	5.889	1.00 32				
ATOM	1746	N	LEU	1709	35.013 33.094	11.041	5.294	1.00 32				
ATOM	1747		LEU	1709	32.378	11.749 10.522	6.245	1.00 31				
ATOM	1748	СВ	LEU	1709	30.973	10.522	5.961	1.00 31				
ATOM	1749	CG	LEU	1709	30.136	9.357	6.565	1.00 28				
ATOM	1750	CD1		1709	30.662	8.059	6.081	1.00 28				
ATOM	1751	CD2		1709	28.705	9.556	6.679 6.437	1.00 27				
ATOM	1752		LEU	1709	32.306	10.317	4.454	1.00 29. 1.00 30.				
MOTA	1753		LEU	1709	32.489	9.202	3.970	1.00 30				
ATOM	1754		PHE	1710	32.043	11.399	3.727	1.00 30				
MOTA	1755		PHE	1710	31.945	11.366	2.279	1.00 30				
ATOM	1756		PHE	1710	31.680	12.768	1.737	1.00 34			٠	
ATOM	1757		PHE	1710	30.310	13.261	2.020					
ATOM	1758	CD1		1710	29.337	12.393	2.495	1.00 37. 1.00 43.				
ATOM	1759	CD2		1710	29.984	14.596	1.838	1.00 43				
ATOM	1760	CEI		1710	28.054	12.834	2.787	1.00 42				
ATOM	1761	CE2		1710	28.698	15.053	2.130	1.00 46.				
ATOM	1762	CZ	PHE	1710	27.733	14.169	2.605	1.00 46				
-				- · — -			2.000	T. OO 40	72			

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ATOM 1763 С PHE 1710 33.196 10.802 1.667 1.00 34.25 1.00 36.09 **ATOM** 1764 0 PHE 1710 0.785 33.133 9.948 MOTA 1765 N LYS 1711 34.324 2.209 1.00 34.37 11.249 10.840 **ATOM** 1766 CA LYS 1711 35.664 1.789 1.00 34.11 ATOM 1767 CB LYS 1711 36.672 11.768 2.476 1.00 37.74 **ATOM** 1768 CG LYS 1711 38.114 11.567 2.119 1.00 43.59 **ATOM** 1769 LYS CD 1711 38.978 12.573 2.857 1.00 46.97 **ATOM** 1770 CE LYS 1711 2.304 40.386 12.575 1.00 51.53 **ATOM** 1771 LYS NZ 1711 11.291 2.603 41.074 1.00 58.84 **ATOM** 1772 С LYS 1711 35.948 9.354 2.103 1.00 33.25 MOTA 1773 0 LYS 1711 36.512 8.641 1.274 1.00 32,22 MOTA 1774 N LEU 1712 35.537 8.894 3.285 1.00 32.62 MOTA 1775 CA . LEU 1712 35.718 7.496 3.667 1.00 31.41 **ATOM** 1776 CB LEU 1712 35.223 7.237 5.106 1.00 29.80 ATOM 1777 CG LEU 1712 36.020 7.889 6.244 1.00 29.22 **ATOM** 1778 CD1 LEU 1712 35.385 7.643 7.608 1.00 24.09 **ATOM** 1779 CD2 LEU 1712 37.437 7.356 6.234 1.00 28.36 MOTA 1780 C LEU 1712 34.939 2.674 6.638 1.00 31.88 **ATOM** 1781 0 LEU 1712 35.452 5.654 2.143 1.00 34.08 ATOM 1782 N LEU 1713 33.700 7.029 2.413 1.00 32.28 32.850 ATOM 1783 CA LEU 1713 1.482 6.305 1.00 35.36 **ATOM** 1784 CB LEU 1713 31.433 6.887 1.485 1.00 38.97 ATOM 1785 CG LEU 1713 30.629 2.730 6.494 1.00 39.56 MOTA 1786 CD1 LEU 1713 29.308 2.768 7.228 1.00 37.14 **ATOM** 1787 CD2 LEU 1713 30.424 4.988 2.748 1.00 37.73 MOTA 1788 LEU C 1713 33.430 6.296 0.070 1.00 36.47 **ATOM** 1789 0 LEU 1713 33.502 5.244 -0.563 1.00 39.32 ATOM 1790 LYS N 1714 33.855 7.455 -0.413 1.00 35.21 MOTA 1791 CA LYS 1714 34.437 7.544 -1.743 1.00 34.55 **ATOM** 1792 CB LYS 1714 8.984 34.812 -2.075 1.00 34.81 MOTA LYS 1793 CG 1714 33.624 9.903 -2.290 1.00 36.55 **ATOM** 1794 CD LYS 1714 32.681 9.372 -3.353 1.00 40.68 MOTA 1795 CE LYS 1714 31.488 10.310 -3.577 1.00 44.87 **ATOM** 1796 NZ LYS 1714 30.611 9.853 -4.701 1.00 50.99 **ATOM** 1797 С LYS 1714 35.671 6.649 -1.856 1.00 35.97 **ATOM** 1798 LYS 0 1714 35.948 6.084 -2.920 1.00 38.11 **ATOM** 1799 N GLU 1715 36.385 6.490 -0.749 1.00 33.65 MOTA 1800 CA GLU 1715 37.582 5.663 -0.729 1.00 34.34 MOTA 1801 CB GLU 1715 38.574 6.221 0.288 1.00 34.90 MOTA 1802 CG GLU 1715 39.032 7.613 -0.110 1.00 42.07 MOTA 1803 CD GLU 1715 39.729 8.405 0.989 1.00 47.94 MOTA 1804 OE1 GLU 1715 39.977 7.870 2.098 1.00 45.03 MOTA OE2 GLU 1805 1715 40.026 9.596 0.709 1.00 51.48 **ATOM** 1806 С GLU 1.00 34.76 1715 37.285 4.191 -0.466 MOTA 1807 0 GLU 1715 38.205 3.384 -0.411 1.00 37.36 **ATOM** 1808 N GLY 1716 36.002 3.848 -0.347 1.00 32.00 MOTA 1809 CA GLY 1716 35.604 2.474 -0.122 1.00 30.49 MOTA 1810 C GLY 1716 35.932 1.937 1.251 1.00 31.32 **ATOM** 1811 0 GLY 1716 36.134 0.738 1.430 1.00 31.83 MOTA 1812 N HIS 1717 35.957 2.822 2.233 1.00 31.55 MOTA 1813 CA HIS 1717 36.265 2.416 3.595 1.00 33.20 MOTA 1814 CB HIS 1717 36.494 3.661 4.452 1.00 37.67

MOTA	1815	CG	HIS	1717	36.786	3.360	5.895	1.00 42.42
ATOM	1816	CD2	HIS	1717	37.957	3.259	6.567	1.00 40.97
MOTA	1817	ND1	HIS	1717	35.789	3.142	6.825	1.00 45.02
MOTA	1818	CE1	HIS	1717	36.333	2.914	8.004	1.00 44.06
MOTA	1819	NE2	HIS	1717	37.645	2.976	7.873	1.00 43.67
MOTA	1820	С	HIS	1717	35.149	1.567	4.201	1.00 31.72
MOTA	1821	0	HIS	1717	33.975	1.816	3.952	1.00 32.12
ATOM	1822	N	ARG	1718	35.529	0.582	5.009	1.00 31.09
MOTA	1823	CA	ARG	1718	34.586	-0.288	5.696	1.00 32.10
ATOM	1824	CB	ARG	1718	34.531	-1.664	5.024	1.00 31.61
ATOM	1825	CG	ARG	1718	34.048	-1.651	3.577	1.00 31.32
ATOM	1826	CD	ARG	1718	32.579	-1.263	3.495	1.00 29.60
ATOM	1827	NE	ARG	1718	32.036	-1.320	2.129	1.00 24.72
ATOM	1828	CZ	ARG	1718	32.103	-0.324	1.243	1.00 22.01
ATOM	1829	NH1	ARG	1718	32.709	0.819	1.554	1.00 19.00
MOTA	1830	NH2	ARG	1718	31.463	-0.444	0.083	1.00 14.18
MOTA	1831	С	ARG	1718	35.042	-0.438	7.164	1.00 33.81
MOTA	1832	О	ARG	1718	36.234	-0.596	7.446	1.00 34.62
MOTA	1833	N	MET	1719	34.084	-0.372	8.085	1.00 33.99
MOTA	1834	CA	MET	1719	34.382	-0.466	9.508	1.00 32.51
MOTA	1835	CB	MET	1719	33.110	-0.246	10.342	1.00 33.51
MOTA	1836	CG	MET	1719	32.513	1.155	10.200	1.00 33.69
ATOM	1837	SD	MET	1719	31.082	1.526	11.251	1.00 37.49
ATOM	1838	CE	MET	1719	29.906	0.373	10.618	1.00 37.62
MOTA	1839	С	MET	1719	35.033	-1.799	9.844	1.00 32.92
ATOM	1840	0	MET	1719	34.900	-2.772	9.098	1.00 33.67
ATOM	1841	N	ASP	1720	35.776	-1.825	10.945	1.00 35.49
ATOM	1842	CA	ASP	1720	36.466	-3.038	11.388	1.00 36.87
ATOM	1843	CB	ASP	1720	37.585	-2.694	12.376	1.00 41.64
ATOM	1844	CG	ASP	1720	38.688	-1.859	11.754	1.00 46.44
ATOM	1845	OD1	ASP	1720	38.507	-1.410	10.604	1.00 52.86
MOTA	1846	OD2	ASP	1720	39.740	-1.650	12.422	1.00 46.76
ATOM	1847	C	ASP	1720	35.516	-4.005	12.053	1.00 34.70
ATOM	1848	О	ASP	1720	34.459	-3.603	12.548	1.00 34.31
MOTA	1849	N	LYS	1721	35.937	-5.265	12.132	1.00 33.39
MOTA	1850	CA	LYS	1721	35.119	-6.297	12.755	1.00 32.68
MOTA	1851	CB	LYS	1721	35.692	-7.690	12.500	1.00 33.55
ATOM	1852	CG	LYS	1721	34.834	-8.791	13.119	1.00 33.62
MOTA	1853	CD	LYS	1721	35.336	-10.158	12.771	1.00 35.77
ATOM	1854	CE	LYS	1721	36.082	-10.747	13.931	1.00 38.73
ATOM	1855	NZ	LYS	1721	36.325	-12.190	13.711	1.00 43.86
MOTA	1856	С	LYS	1721	35.034	-6.107	14.240	1.00 34.61
ATOM	1857	O	LYS	1721	36.057	-5.944	14.905	1.00 37.05
ATOM	1858	N	PRO	1722	33.808	-6.092	14.781	1.00 36.16
ATOM	1859	CD	PRO	1722	32.518	-6.062	14.066	1.00 34.73
ATOM	1860	CA	PRO	1722	33.611	-5.926	16.222	1.00 37.84
ATOM	1861	СВ	PRO	1722	32.095	-6.017	16.360	1.00 37.19
ATOM	1862	CG	PRO	1722	31.607	-5.448	15.073	1.00 36.00
ATOM	1863	С	PRO	1722	34.266	-7.109	16.950	1.00 39.95
ATOM	1864	0	PRO	1722	34.340	-8.218	16.406	1.00 38.82
ATOM	1865	N	SER	1723	34.783	-6.884	18.150	1.00 42.36
ATOM	1866	CA	SER	1723	35.359	-7.995	18.890	1.00 45.70
							20.000	2.00 45.70

ATOM	1867	CB	SER	1723	36.170 -7.511	20.093	1.00 47.50
MOTA	1868	OG	SER	1723	35.341 -6.964	21.100	1.00 55.28
ATOM	1869	С	SER	1723	34.136 -8.784	19.346	1.00 46.70
ATOM	1870	0	SER	1723	33.037 -8.224	19.477	1.00 47.27
ATOM	1871	N	ASN	1724	34.296 -10.081	19.559	1.00 47.84
ATOM	1872	CA	ASN	1724	33.174 -10.900	19.992	1.00 51.26
MOTA	1873	CB	ASN	1724	32.620 -10.361	21.330	1.00 57.15
ATOM	1874	CG	ASN	1724	33.732 -10.088	22.365	1.00 61.53
ATOM	1875	OD1	ASN	1724	34.565 -10.955	22.646	1.00 64.13
ATOM	1876	ND2	ASN	1724	33.763 -8.867	22.912	1.00 61.69
ATOM	1877	C	ASN	1724	32.101 -10.916	18.873	1.00 50.72
ATOM	1878	0	ASN	1724	30.925 -10.617	19.089	1.00 52.63
ATOM	1879	N	CYS	1725	32.564 -11.193	17.663	1.00 48.01
ATOM	1880	CA	CYS	1725	31.719 -11.295	16.478	1.00 45.16
ATOM	1881	CB	CYS	1725	31.603 -9.929	15.788	1.00 44.77
ATOM	1882	SG	CYS	1725	30.605 -9.929	14.272	1.00 40.74
ATOM	1883	C	CYS	1725	32.421 -12.308	15.570	1.00 41.51
ATOM	1884	0	CYS	1725	33.639 -12.236	15.397	1.00 42.47
ATOM	1885	N	THR	1726	31.677 -13.289	15.064	1.00 37.54
MOTA	1886	CA	THR	1726	32.268 -14.313	14.202	1.00 35.03
ATOM	1887	CB	THR	1726	31.308 -15.500	13.993	1.00 31.87
ATOM	1888	OG1	THR	1726	30.074 -15.042	13.406	1.00 32.84
MOTA	1889	CG2	THR	1726	31.017 -16.160	15.306	1.00 29.78
ATOM	1890	С	THR	1726	32.678 -13.770	12.845	1.00 34.76
MOTA	1891	0	THR	1726	32.180 -12.729	12.415	1.00 38.22
MOTA	1892	N	ASN	1727	33.596 -14.450	12.175	1.00 32.47
ATOM	1893	CA	ASN	1727	34.009 -14.024	10.842	1.00 34.75
MOTA	1894	CB	ASN	1727	35.167 -14.872	10.308	1.00 39.77
ATOM	1895	CG	asn	1727	36.464 -14.591	11.026	1.00 46.09
MOTA	1896	OD1	ASN	1727	37.019 -13.495	10.933	1.00 49.54
MOTA	1897	ND2	ASN	1727	36.961 -15.585	11.749	1.00 50.04
MOTA	1898	С	ASN	1727	32.825 -14.147	9.905	1.00 33.38
ATOM	1899	0	ASN	1727	32.726 -13.405	8.929	1.00 34.10
ATOM	1900	N	GLU	1728	31.916 -15.065	10.224	1.00 32.01
ATOM	1901	CA	GLU	1728	30.707 -15.310	9.418	1.00 30.41
MOTA	1902	CB	GLU	1728	30.010 -16.580	9.917	1.00 32.27
ATOM	1903	CG	GLU	1728	28.811 -17.034	9.094	1.00 31.55
ATOM	1904	CD	GLU	1728	28.251 -18.369	9.577	1.00 36.38
ATOM	1905	OE1		1728	28.415 -18.694	10.777	1.00 38.35
MOTA	1906		GLU	1728	27.632 -19.086	8.758	1.00 36.34
ATOM		C	GLU	1728	29.749 -14.119	9.468	1.00 29.40
ATOM	1908	0	GLU	1728	29.231 -13.679	8.438	1.00 26.23
MOTA	1909	N	LEU	1729	29.520 -13.610	10.672	1.00 29.19
ATOM	1910	CA	LEU	1729	28.645 -12.462	10.849	1.00 30.26
MOTA	1911	CB	LEU	1729	28.215 -12.343	12.310	1.00 30.74
MOTA	1912	CG	LEU	1729	27.198 -13.410	12.721	1.00 31.27
ATOM	1913	CD1		1729	27.013 -13.377	14.226	1.00 33.65
ATOM	1914	CD2		1729	25.865 -13.161	12.010	1.00 26.16
MOTA	1915	С	LEU	1729	29.269 -11.161	10.335	1.00 28.79
MOTA	1916	0	LEU	1729	28.548 -10.255	9.914	1.00 30.60
MOTA	1917	N	TYR	1730	30.594 -11.069	10.363	1.00 26.64
ATOM	1918	CA	TYR	1730	31.281 -9.881	9.844	1.00 26.47

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MOTA	1919	CB	TYR	1730	32.742	-9.869	10.298	1.00 24.31
ATOM	1920	CG	TYR	1730	33.512	-8.670	9.805	1.00 25.61
ATOM	1921	CD1	TYR	1730	33.029	-7.373	10.016	1.00 25.68
ATOM	1922	CE1	TYR	1730	33.691	-6.264	9.496	1.00 23.70
ATOM	1923	CD2	TYR	1730	34.688	-8.826	9.067	1.00 24.48
ATOM	1924	CE2	TYR	1730	35.361	-7.719	8.537	1.00 22.61
ATOM	1925	CZ	TYR	1730	34.856	-6.445	8.748	1.00 24.41
MOTA	1926	OH	TYR	1730	35.476	-5.354	8.176	1.00 24.37
ATOM	1927	С	TYR	1730	31.186	-9.902	8.301	1.00 26.06
ATOM	1928	0	TYR	1730	30.981	-8.881	7.651	1.00 23.68
ATOM	1929	N	MET	1731		-11.084	7.727	1.00 26.60
ATOM	1930	CA	MET	1731	•	-11.270	6.299	1.00 29.90
ATOM	1931	CB	MET	1731		-12.740	5.968	1.00 38.39
ATOM	1932	CG	MET	1731		-13.157	4.577	1.00 52.98
MOTA	1933	SD	MET	1731		-14.831	4.216	1.00 69.59
MOTA	1934	CE	MET	1731		-14.506	2.727	1.00 66.05
ATOM	1935	С	MET	1731		-10.819	5.840	1.00 29.05
MOTA	1936	0	MET	1731		-10.194	4.791	1.00 30.94
ATOM	1937	N	MET	1732		-11.134	6.633	1.00 29.40
ATOM	1938	CA	MET	1732		-10.743	6.328	1.00 26.97
MOTA	1939	CB	MET	1732		-11.293	7.398	1.00 25.73
MOTA	1940	CG	MET	1732	25.068	-10.984	7.156	1.00 26.01
ATOM	1941	SD	MET	1732	23.980	-11.637	8.407	1.00 26.97
ATOM	1942	CE	MET	1732	23.773	-13.354	7.798	1.00 21.23
ATOM	1943	C	MET	1732	27.387	-9.220	6.271	1.00 27.49
ATOM	1944	0	MET	1732	26.778	-B.661	5.361	1.00 29.17
MOTA	1945	N	MET	1733	27.982	-8.550	7.259	1.00 27.79
ATOM	1946	CA	MET	1733	28.001	-7.090	7.293	1.00 27.41
ATOM	1947	CB	MET	1733	28.797	-6.587	8.484	1.00 28.84
ATOM	1948	CG	MET	1733 .	28.153	-6.761	9.829	1.00 32.18
MOTA	1949	SD	MET	1733	29.300	-6.248	11.127	1.00 32.77
ATOM	1950	CE	MET	1733	28.850	-7.423	12.399	1.00 33.03
MOTA	1951	С	MET	1733	28.711	-6.599	6.035	1.00 28.54
ATOM	1952	0	MET	1733	28.250	-5.680	5.357	1.00 30.69
ATOM	1953	N	ARG	1734	29.865	-7.194	5.751	1.00 28.59
ATOM	1954	CA	ARG	1734	30.650	-6.831	4.571	1.00 29.53
ATOM	1955	CB	ARG	1734	31.970	-7.609	4.531	1.00 28.74
ATOM	1956	CG	ARG	1734	32.944	-7.245	5.638	1.00 26.75
ATOM	1957	CD	ARG	1734	33.158	-5.755	5.702	1.00 26.58
ATOM	1958	NE	ARG	1734	33.825	-5.288	4.499	1.00 34.72
ATOM	1959	CZ	ARG	1734	35.139	-5.360	4.306	1.00 37.67
ATOM	1960	NH1		1734	35.927	-5.867	5.251	1.00 40.46
MOTA	1961	NH2	ARG	1734	35.663	-4.986	3.147	1.00 38.11
MOTA	1962	С	ARG	1734	29.855	-7.051	3.294	1.00 28.03
ATOM	1963	0	ARG	1734	29.958	-6.260	2.359	1.00 27.22
ATOM	1964	N	ASP	1735	29.071	-8.130	3.260	1.00 27.81
MOTA	1965	CA	ASP	1735	28.212	-8.436	2.103	1.00 27.27
ATOM	1966	CB	ASP	1735	27.608	-9.835	2.216	1.00 28.62
ATOM	1967	CG	ASP	1735	28.638	-10.932	2.075	1.00 30.15
MOTA	196B	OD1		1735	29.745	-10.663	1.553	1.00 31.23
ATOM	1969	OD2	ASP	1735	28.354	-12.070	2.501	1.00 32.00
ATOM	1970	С	ASP	1735	27.099	-7.400	1.971	1.00 24.78

ATOM	1971	0	ASP	1735	26.714	-7.068	0.852	1.00 24.52
ATOM	1972	N	CYS	1736	26.590	-6.908	3.104	1.00 24.10
MOTA	1973	CA	CYS	1736	25.530	-5.871	3.140	1.00 25.20
ATOM	1974	CB	CYS	1736	24.965	-5.679	4.569	1.00 23.85
MOTA	1975	SG	CYS	1736	23.898	-7.030	5.143	1.00 18.77
MOTA	1976	C	CYS	1736	26.042	-4.520	2.611	1.00 23.39
ATOM	1977	0	CYS	1736	25.276	-3.718	2.070	1.00 21.76
MOTA	1978	N	TRP	1737	27.348	-4.303	2.743	1.00 23.53
ATOM	1979	CA	TRP	1737	27.988	-3.072	2.302	1.00 21.57
ATOM	1980	CB	TRP	1737	29.026	-2.631	3.314	1.00 18.82
ATOM	1981	CG	TRP	1737	28.485	-2.418	4.686	1.00 19.89
ATOM	1982	CD2	TRP	1737	29.194	-2.609	5.913	1.00 22.39
ATOM	1983	CE2	TRP	1737	28.329	-2.213	6.959	1.00-21.78
ATOM	1984	CE3	TRP	1737	30.478	-3.083	6.238	1.00 23.52
MOTA	1985	CD1	TRP	1737	27.248	-1.932	5.022	1.00 19.40
ATOM	1986	NE1	TRP	1737	27.147	-1.805	6.383	1.00 21.52
MOTA	1987	CZ2	TRP	1737	28.705	-2.270	8.319	1.00 21.85
MOTA	1988	CZ3	TRP	1737	30.857	-3.134	7.583	1.00 25.30
ATOM	1989	CH2	TRP	1737	29.972	-2.728	8.604	1.00 26.17
ATOM	1990	С	TRP	1737	28.673	-3.226	0.956	1.00 24.49
ATOM	1991	0	TRP	1737	29.648	-2.519	0.670	1.00 25.09
ATOM	1992	N	HIS	1738	28.203	~4.170	0.136	1.00 25.12
MOTA	1993	CA	HIS	1738	28.808	-4.341	-1.172	1.00 22.90
ATOM	1994	CB	HIS	1738	28.163	-5.497	-1.928	1.00 23.14
ATOM	1995	CG	HIS	1738	29.017	-6.013	-3.051	1.00 23.26
MOTA	1996	CD2	HIS	1738	29.550	-5.380	-4.129	1.00 23.78
MOTA	1997	ND1	HIS	1738	29.492	-7.308	-3.104	1.00 24.91
MOTA	1998	CE1	HIS	1738	30.286	-7.445	-4.156	1.00 25.29
MOTA	1999	NE2	HIS	1738	30.341	-6.288	-4.794	1.00 26.99
MOTA	2000	С	HIS	1738	28.670	-3.024	-1.958	1.00 22.92
MOTA	2001	0	HIS	1738	27.615	-2.381	-1.933	1.00 20.27
ATOM	2002	N	ALA	1739	29.752	-2.608	-2.607	1.00 24.30
ATOM	2003	CA	ALA	1739	29.762	-1.378	-3.385	1.00 23.70
ATOM	2004	CB	ALA	1739	31.079	-1.234	-4.076	1.00 25.24
ATOM	2005	С	ALA	1739	28.645	-1.391	-4.416	1.00 25.37
MOTA	2006	0	ALA	1739	27.955	-0.391	-4.606	1.00 27.86
ATOM	2007	N	VAL	1740	28.507	-2.521	-5.102	1.00 23.97
ATOM	2008	CA	VAL	1740	27.481	-2.700	-6.121	1.00 24.64
ATOM	2009	CB	VAL	1740	27.966	-3.698	-7.206	1.00 26.39
ATOM	2010		VAL	1740	27.013	-3.757	-8.360	1.00 22.65
ATOM	2011		VAL	1740	29.308	-3.260	-7.720	1.00 27.43
MOTA	2012	C	VAL	1740	26.170	-3.209	-5.481	1.00 23.97
ATOM	2013	0	VAL	1740	26.126	-4.347	-4.97B	1.00 24.14
ATOM	2014	N	PRO	1741	25.090	-2.397	-5.545	1.00 22.77
ATOM	2015	CD	PRO	1741	25.074	-1.093	-6.237	1.00 17.82
ATOM	2016	CA	PRO	1741	23.763	-2.695	-4.980	1.00 23.22
ATOM	2017	CB	PRO	1741	22.891	-1.554	-5.526	1.00 18.19
ATOM	2018	CG	PRO	1741	23.866	-0.419	-5.647	1.00 15.09
ATOM	2019	C	PRO	1741	23.189	-4.074	-5.343	1.00 23.26
ATOM	2020	0	PRO	1741	22.700	-4.788	-4.462	1.00 22.42
ATOM	2021	N	SER	1742	23.335	-4.473	-6.615	1.00 23.49
ATOM	2022	CA	SER	1742	22.826	-5.754	-7.119	1.00 23.17

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MOTA 2023 CB SER 1742 22.956 -5.808 -8.641 1.00 23.67 2024 **ATOM** SER OG 1742 24.324 -5.891 -9.023 1.00 26,64 MOTA 2025 С SER 1742 23.524 -6.984 -6.545 1.00 23.09 MOTA 2026 0 SER 1742 22.993 -8.104 -6.603 1.00 21.90 MOTA 2027 N GLN 1743 24.719 -6.782 -5.997 1.00 23.62 **ATOM** 2028 CA GLN 1743 25.466 -7.895 -5.416 1.00 23.26 MOTA 2029 CB GLN 1743 26.953 -7.754 -5.702 1.00 24.32 MOTA 2030 CG GLN 1743 27.255 -7.828 -7.170 1.00 23.04 MOTA 2031 CD GLN 1743 26.684 -9.076 -7.810 1.00 24.83 MOTA 2032 OE1 GLN 1743 -7.584 27.176 -10.178 1.00 21.07 MOTA 2033 NE2 GLN 1743 25.647 -8.907 -8.625 1.00 22.66 MOTA 2034 С GLN 1743 25.227 -8.121 -3.927 1.00 23.85 MOTA GLN 1743 2035 0 25.744 -9.083 -3.366 1.00 25.36 MOTA 2036 N ARG 1744 24.458 -7.240 -3.290 1.00 22.69 MOTA 2037 CA ARG 1744 24.155 -7.395 -1.868 1.00 21.65 MOTA 2038 CB ARĢ 1744 23.635 -6.087 -1.277 1.00 21.22 MOTA 2039 CG ARG 1744 24.623 -4.962 -1.342 1.00 21.63 MOTA 2040 CD ARG 1744 24.013 -3.656 -0.863 1.00 19.06 ATOM 2041 NE ARG 1744 24.869 -2.563 -1.318 1.00 24.44 CZATOM 2042 ARG 1744 24.461 -1.322 -1.564 1.00 22.49 ATOM 2043 NH1 ARG 1744 23.184 -0.972 -1.378 1.00 18.95 ATOM 2044 NH2 ARG 1744 25.337 -0.438 -2.034 1.00 22.19 MOTA 2045 C ARG 1744 23.095 -8.470 -1.712 1.00 22.45 ATOM 2046 0 ARG 1744 22.363 -8.772 -2.654 1.00 25.62 MOTA 2047 N PRO 1745 23.065 -9.139 -0.559 1.00 21.78 MOTA 2048 CD PRO 1745 24.025 -9.114 0.563 1.00 21.02 22.057 -10.175 -0.362 1.00 20.99 MOTA 2049 CA PRO 1745 22.532 -10.879 MOTA 2050 CB PRO 1745 0.919 1.00 21.12 MOTA 2051 CG -9.777 PRO 1745 1.676 1.00 19.86 23.240 MOTA 2052 C PRO 1745 20.726 -9.485 -0.146 1.00 22.18 MOTA. 2053 PRO 1745 0 20.680 -8.281 0.128 1.00 23.04 MOTA 2054 N THR 1746 19.646 -10.236 -0.297 1.00 19.31 MOTA 2055 CA THR 1746 18.335 -9.689 -0.085 1.00 19.12 MOTA 2056 CB THR 1746 17.307 -10.334 -1.045 1.00 19.86 MOTA 2057 OG1 THR 1746 17.299 -11.763 -0.886 1.00 22.54 ATOM 2058 CG2 THR 1746 17.668 -10.002 -2.479 1.00 22.97 MOTA 2059 C THR 17.961 -9.975 1746 1.367 1.00 19.91 MOTA 2060 O THR 1746 18.676 -10.711 2.058 1.00 19.93 ATOM 2061 N PHE 1747 16.884 -9.381 1.855 1.00 21.80 MOTA 2062 CA PHE 1747 16.456 -9.678 3.224 1.00 23.46 MOTA 2063 CB PHE 1747 15.353 -8.720 3.686 1.00 21.84 MOTA 2064 CG PHE 1747 15.872 -7.368 4.082 1.00 24.84 MOTA 2065 CD1 PHE 1747 16.627 -7.207 5.237 1.00 22.23 MOTA 2066 CD2 PHE 1747 15.611 -6.248 3.293 1.00 22.97 MOTA 2067 CE1 PHE 1747 17.124 -5.944 5.598 1.00 19.42 MOTA 2068 CE2 PHE 1747 16.111 -4.991 3.646 1.00 17.14 MOTA 2069 CZ PHE 1747 16.862 -4.846 4.801 1.00 18.02 MOTA 2070 15.992 -11.133 С PHE 1747 3.295 1.00 22.28 MOTA 2071 PHE 0 1747 16.189 -11.796 4.304 1.00 23.76 MOTA 2072 N LYS 1748 15.430 -11.632 2.199 1.00 23.46 MOTA 2073 CA LYS 1748 14.971 -13.014 2.140 1.00 25.84 **ATOM** 2074 LYS 1748 CB 14.344 -13.327 0.782 1.00 26.89

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MOTA 2075 CG LYS 1748 14.061 -14.793 0.583 1.00 31.07 MOTA 2076 CD LYS 1748 13.714 -15.064 -0.861 1.00 37.82 **ATOM** 2077 CE LYS 1748 13.231 -16.493 -1.068 1.00 44.36 **ATOM** 2078 NZ LYS 1748 12.027 -16.782 -0.235 1.00 50.16 MOTA 2079 С LYS 1748 16.160 -13.949 2.393 1.00 27.27 **ATOM** 2080 0 LYS 1748 16.067 -14.877 3.202 1.00 27.87 ATOM 2081 N GLN 1749 17.288 -13.674 1.730 1.00 25.64 **ATOM** 2082 CA GLN 1749 18.507 -14.457 1.903 1.00 24.32 **ATOM** 2083 CB GLN 1749 19.608 -13.938 0.983 1.00 28.87 MOTA 2084 CG GLN 1749 19.343 -14.049 -0.496 1.00 36.24 MOTA 2085 CD GLN 1749 20.437 -13.374 -1.318 1.00 41.30 **ATOM** 2086 OE1 GLN 1749 20.173 -12.422 -2.044 1.00 38.35 MOTA 2087 NE₂ GLN 1749 -- 21.683 -- 13.861 -1.190 1.00 45.38 MOTA 2088 C GLN 1749 19.002 -14.310 1.00 22.89 3.346 MOTA 2089 O GLN 1749 19.302 -15.305 4.008 1.00 22.55 ATOM 2090 N LEU 1750 19.114 -13.064 3.813 1.00 20.89 ATOM 2091 CA LEU 1750 19.570 -12.776 5.167 1.00 21.44 ATOM 2092 CB LEU 1750 19.471 -11.282 5.462 1.00 19.53 **ATOM** 2093 CG LEU 1750 20.432 -10.400 4.663 1.00 19.14 **ATOM** 2094 CD1 LEU 1750 20.069 -8.919 4.816 1.00 14.53 ATOM 2095 CD2 LEU 1750 21.863 -10.685 5.106 1.00 16.18 MOTA 2096 С LEU 1750 18.776 -13.538 6.208 1.00 22.98 MOTA 2097 0 LEU 1750 19.335 -14.057 1.00 23.12 7.183 MOTA 2098 N VAL 1751 17.465 -13.586 6.020 1.00 23.48 **ATOM** 2099 CA VAL 1751 16.610 -14.292 6.945 1.00 23.21 MOTA 2100 CB VAL 1751 15.132 -14.075 6.590 1.00 20.94 **ATOM** 2101 CG1 VAL 1751 14.268 -15.008 7.375 1.00 21.67 MOTA 2102 CG2 VAL 1751 14.730 -12.649 6.929 1.00 20.32 MOTA 2103 C VAL 1751 16.974 -15.774 6.990 1.00 26.13 **ATOM** 2104 O VAL 1751 17.030 -16.379 8.058 1.00 26.35 MOTA 2105 GLU 5.831 N 1752 17.260 -16.348 1.00 30.05 **ATOM** 2106 CA GLU 1752 17.632 -17.747 5.778 1.00 32.54 ATOM 2107 CB GLU 17.695 -18.221 1752 4.338 1.00 38.54 **ATOM** 2108 CG GLU 1752 16.322 -18.226 3.673 1.00 50.06 MOTA 2109 CD GLU 1752 16.333 -18.759 2.247 1.00 56.55 MOTA 2110 OE1 GLU 1752 15.365 -18.480 1.507 1.00 61.63 ATOM 2111 OE2 GLU 1752 17.303 -19.466 1.875 1.00 59.57 **ATOM** 2112 С GLU 1752 18.974 -17.965 6.486 1.00 31.62 **ATOM** 2113 0 GLU 1752 19.113 -18.858 7.322 1.00 29.63 **ATOM** 2114 N ASP 1753 19.938 -17.103 6.193 1.00 30.74 MOTA ASP 2115 CA 1753 21.246 -17.211 6.807 1.00 31.00 MOTA 2116 CB ASP 1753 22.209 -16.181 6.203 1.00 31.47 **ATOM** 2117 CG ASP 1753 22.445 -16.390 4.710 1.00 35.82 MOTA 2118 OD1 ASP 1753 22.396 -17.549 4.248 1.00 36.78 MOTA 2119 OD2 ASP 1753 22.671 -15.396 3.992 1.00 41.04 **ATOM** 21.158 -17.058 2120 C ASP 1753 8.314 1.00 28.94 **ATOM** 2121 21.597 -17.933 0 ASP 1753 9.059 1.00 29.91 ATOM 2122 N LEU 1754 20.526 -15.984 8.764 1.00 28.33 MOTA 2123 CA LEU 1754 20.386 -15.731 10.199 1.00 26.88 MOTA 2124 CB LEU 1754 19.724 -14.372 10.457 1.00 19.82 MOTA 2125 CG LEU 1754 20.737 -13.269 10.154 1.00 20.90 MOTA 2126 CD1 LEU 1754 20.074 -11.886 9.995 1.00 14.83

ATOM	2127	CD2	LEU	1754	21.831	-13.308	11.240	1.00 16.39
MOTA	2128	С	LEU	1754	19.645	-16.861	10.896	1.00 29.18
MOTA	2129	0	LEU	1754	20.030	-17.262	11.986	1.00 30.55
MOTA	2130	N	ASP	1755	18.638	-17.421	10.238	1.00 31.65
ATOM	2131	CA	ASP	1755	17.892	-18.517	10.822	1.00 31.78
MOTA	2132	CB	ASP	1755	16.723	-18.900	9.928	1.00 34.57
ATOM	2133	CG	ASP	1755	15.876	-19.997	10.533	1.00 38.29
MOTA	2134	OD1	ASP	1755	15.410	-19.844	11.677	1.00 45.68
ATOM	2135	OD2	ASP	1755	15.685	-21.031	9.878	1.00 43.05
MOTA	2136	С	ASP	1755	18.801	-19.713	11.034	1.00 33.50
MOTA	2137	0	ASP	1755	18.665	-20.428	12.025	1.00 34.39
MOTA	2138	N	ARG	1,756	19.738	-19.907	10.107	1.00 35.51
MOTA	2139	CA	ARG	1756	20.700	-21.004	10.169	1.00 35.33
ATOM	2140	CB	ARG	1756	21.417	-21.125	8.825	1.00 38.41
MOTA	2141	CG	ARG	1756	22.522	-22.181	8.759	1.00 40.99
MOTA	2142	CD	ARG	1756	23.181	-22.223	7.376	1.00 44.60
MOTA	2143	NE	ARG	1756	23.676	-20.917	6.916	1.00 49.55
MOTA	2144	CZ	ARG	1756	24.795	-20.338	7.349	1.00 53.56
ATOM	2145	NH1	ARG	1756	25.556	-20.937	8.266	1.00 53.25
MOTA	2146	NH2	ARG	1756	25.165	-19.163	6.853	1.00 55.72
ATOM	2147	C	ARG	1756	21.719	-20.754	11.275	1.00 35.01
MOTA	2148	0	ARG	1756	22.000	-21.632	12.088	1.00 34.86
MOTA	2149	N	ILE	1757	22.244	-19.536	11.314	1.00 35.06
MOTA	2150	CA	ILE	1757	23.242	-19.153	12.302	1.00 35.25
ATOM	2151	CB	ILE	1757	23.847	-17.753	11.984	1.00 34.59
ATOM	2152	CG2	ILE	1757	24.915	-17.401	12.995	1.00 32.98
MOTA	2153	CG1	ILE	1757	24.481	-17.757	10.586	1.00 33.64
MOTA	2154	CD1	ILE	1757	24.812	-16.387	10.032	1.00 28.79
MOTA	2155	С	ILE	1757	22.673	-19.182	13.716	1.00 36.74
MOTA	2156	0	ILE	1757	23.283	-19.764	14.601	1.00 36.60
ATOM	2157	N	VAL	1758	21.489	-18.608	13.917	1.00 39.16
MOTA	2158	CA	VAL	1758	20.854	-18.589	15.243	1.00 41.06
MOTA	2159	CB	VAL	1758	19.378	-18.104	15.165	1.00 38.77
ATOM	2160	CG1	VAL	1758	18.715	-18.183	16.530	1.00 38.72
MOTA	2161	CG2	VAL	1758	19.309	-16.670	14.651	1.00 39.49
MOTA	2162	С	VAL	1758	20.885	-19.986	15.850	1.00 43.92
ATOM	2163	0	VAL	1758	21.403	-20.182	16.954	1.00 46.90
ATOM	2164	N	ALA	1759	20.370	-20.957	15.098	1.00 43.96
MOTA	2165	CA	ALA	1759	20.325	-22.354	15.528	1.00 43.47
MOTA	2166	CB	ALA	1759	19.653		14.460	1.00 42.26
MOTA	2167	C	ALA	1759	21.693.	-22.953	15.890	1.00 44.02
MOTA	2168	0	ALA	1759	21.780		16.697	1.00 45.94
MOTA	2169	N	LEU	1760	22.750	-22.465	15.255	1.00 45.07
ATOM	2170	CA	LEU	1760	24.095	-22.949	15.514	1.00 46.72
ATOM	2171	CB	LEU	1760	24.899	-22.900	14.225	1.00 48.22
ATOM	2172	CG	LEU	1760	24.279	-23.645	13.053	1.00 51.98
ATOM	2173	CD1		1760	25.016		11.778	1.00 56.19
ATOM	2174	CD2		1760	24.327	-25.136	13.313	1.00 52.82
ATOM	2175	С	LEU	1760	24.811		16.578	1.00 47.59
MOTA	2176	0	LEU	1760	25.935		16.986	1.00 44.63
ATOM	2177	N	THR	1761	24.181	-21.031	17.004	1.00 49.32
ATOM	2178	CA	THR	1761	24.791	-20.166	17.987	1.00 50.15

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24.309 -18.707 MOTA 2179 CB THR 1761 17.811 1.00 49.78 **ATOM** 2180 OG1 THR 1761 24.650 -18.262 16.489 1.00 49.83 MOTA 2181 CG2 THR 1.00 49.37 1761 24.997 -17.793 18.809 C MOTA 2182 THR 1761 24.643 -20.655 19.426 1.00 51.84 MOTA 2183 0 THR 1761 23.565 -21.064 19.866 1.00 51.38 MOTA 2184 N SER 1762 25.761 -20.622 20.143 1.00 53.45 1762 MOTA 2185 CA SER 25.835 -21.042 21.533 1.00 53.79 MOTA 2186 CB 1762 SER 27.301 -21.039 21.969 1.00 58.33 MOTA 2187 OG SER 27.502 -21.759 1762 23.173 1.00 63.27 MOTA 2188 C SER 1762 25.033 -20.081 22.403 1.00 50.43 MOTA 2189 0 SER 1762 25.193 -18.856 22.301 1.00 48.42 **ATOM** 2190 N ALA 79.680 25.808 461 14.502 1.00 57.40 MOTA 2191 CA ALA 79.609 24.651 13.610 461 1.00 53.47 **ATOM** 2192 CB ALA 78.307 23.875 13.860 461 1.00 54.34 MOTA 2193 C ALA 79.707 25.105 12.151 461 1.00 49.53 MOTA 2194 O ALA 461 79.739 24.289 11.243 1.00 48.04 **ATOM** 2195 N ALA 79.814 462 26.417 11.957 1.00 46.57 ATOM 2196 CA ALA 462 79.919 27.014 10.634 1.00 43.66 MOTA 2197 CB ALA 80.034 28.532 10.750 462 1.00 43.87 **ATOM** 2198 С ALA 81.074 462 26.461 9.806 1.00 39.75 ATOM 2199 0 ALA 462 80.869 26.036 8.673 1.00 36.18 ATOM 2200 N TYR 82.279 463 26.449 10.383 1.00 37.82 MOTA 2201 CA TYR 463 83.477 25.959 9.686 1.00 36.88 MOTA 2202 CB 84.615 26.968 TYR 463 9.765 1.00 39.12 MOTA 2203 CGTYR 463 84.372 28.176 8.894 1.00 45.68 MOTA 2204 CD1 TYR 463 84.071 29.422 9.456 1.00 46.07 MOTA 2205 CE1 TYR 463 83.783 30.518 8.652 1.00 48.07 MOTA 2206 CD2 TYR 84.384 28.064 463 7.501 1.00 47.80 MOTA 2207 CE2 TYR 463 84.096 29.154 6.690 1.00 45.55 MOTA 2208 CZTYR 463 83.796 30.372 7.271 1.00 47.44 MOTA 2209 OH TYR 463 83.491 31.442 6.476 1.00 49.77 MOTA 2210 С TYR 463 83.988 24.579 10.024 1.00 34.97 MOTA 2211 0 463 84.605 TYR 23.947 9.175 1.00 35.48 **ATOM** 2212 N GLU 464 83.761 24.109 11.244 1.00 34.33 MOTA 2213 CA GLU 464 84.224 22.769 11.630 1.00 36.96 **ATOM** 2214 CB GLU 464 85.725 22.790 11.901 1.00 41.01 MOTA 2215 CG GLU 464 86.123 23.764 12.991 1.00 45.91 **ATOM** 2216 CD GLU 24.009 464 87.619 13.075 1.00 53.97 MOTA 2217 OE1 GLU 464 88.013 24.922 13.835 1.00 58.84 MOTA 2218 OE2 GLU 464 88.400 23.311 12.383 1.00 56.78 MOTA 2219 C GLU 464 83.517 22.294 12.875 1.00 34.98 MOTA 2220 0 GLU 464 83.252 23.106 13.763 1.00 35.30 MOTA 2221 N LEU 465 83.193 21.003 12.939 1.00 33.52 **ATOM** 2222 CA LEU 465 82.527 20.449 14.121 1.00 35.65 MOTA 2223 CB LEU 465 81.520 19.348 13.762 1.00 32.97 **ATOM** 2224 CG LEU 465 80.488 19.538 12.651 1.00 33.16 ATOM 2225 CD1 LEU 465 79.356 18.544 12.911 1.00 27.30 ATOM 2226 CD2 LEU 465 79.983 20.981 12.596 1.00 29.96 **ATOM** 2227 С LEU 465 83.572 19.862 15.058 1.00 38.14 MOTA 2228 0 LEU 465 84.707 19.573 14.642 1.00 35.58 ATOM 2229 N PRO 466 83.215 19.684 16.338 1.00 39.91 **ATOM** 2230 CDPRO 466 81.929 20.073 16.942 1.00 42.38

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MOTA	2231	CA	PRO	466	84.118	19.126	17.348	1.00 40.82
ATOM	2232	CB	PRO	466	83.264	19.131	18.611	1.00 41.62
ATOM	2233	CG	PRO	466	82.327	20.294	18.380	1.00 45.42
ATOM	2234	С	PRO	466	84.475	17.707	16.976	1.00 41.29
ATOM	2235	0	PRO	466	83.681	16.996	16.361	1.00 40.64
MOTA	2236	N	GLU	467	85.664	17.292	17.370	1.00 43.54
MOTA	2237	CA	GLU	467	86.106	15.950	17.065	1.00 47.01
MOTA	2238	CB	GLU	467	87.569	15.955	16.627	1.00 50.95
ATOM	2239	CG	GLU	467	88.000	14.641	15.990	1.00 59.47
ATOM	2240	CD	GLU	467	89.372	14.700	15.334	1.00 63.95
MOTA	2241	OE1	GLU	467	90.123	15.688	15.538	1.00 62.08
MOTA	2242		GLU	467	89.697	13.736	14.606	1.00 66.76
MOTA	2243	.G	GLU	467	85.892	14.993	18.233	1.00 44.81
MOTA	2244	0	GLU	467	85.988	15.386	19.397	1.00 45.53
ATOM	2245	N	ASP	468	85.572	13.751	17.906	1.00 43.85
ATOM	2246	CA	ASP	468	85.357	12.708	18.903	1.00 43.44
ATOM	2247	CB	ASP	468	83.872	12.582	19.247	1.00 43.33
MOTA	2248	CG	ASP	468	83.611	11.659	20.420	1.00 44.52
MOTA	2249	OD1	ASP	468	82.452	11.613	20.888	1.00 48.19
MOTA	2250	QD2	ASP	468	84.557	10.985	20.877	1.00 42.43
MOTA	2251	С	ASP	468	85.887	11.411	18.299	1.00 42.37
MOTA	2252	0	ASP	468	85.158	10.644	17.669	1.00 43.22
ATOM	2253	N	PRO	469	87.194	11.182	18.433	1.00 40.72
ATOM	2254	CD	PRO	469	88.167	12.102	19.045	1.00 40.30
MOTA	2255	CA	PRO	469	87.861	9.992	17.909	1.00 39.00
ATOM	2256	CB	PRO	469	89.228	10.078	18.570	1.00 39.03
ATOM	2257	CG	PRO	469	89.484	11.564	18.551	1.00 38.11
MOTA	2258	С	PRO	469	87.173	8.663	18.229	1.00 39.37
MOTA	2259	0	PRO	469	87.235	7.718	17.442	1.00 39.27
ATOM	2260	N	ARG	470	86.497	8.596	19.371	1.00 39.93
MOTA	2261	CA	ARG	470	85.814	7.374	19.770	1.00 42.32
ATOM	2262	CB	ARG	470	85.030	7.614	21.062	1.00 46.12
ATOM	2263	CG	ARG	470	85.766	8.370	22.149	1.00 50.76
MOTA	2264	CD	ARG	470	84.839	8.592	23.344	1.00 52.76
ATOM	2265	NE	ARG	470	83.649	9.362	22.991	1.00 54.47
ATOM	2266	CZ	ARG	470	82.770	9.823	23.873	1.00 59.36
ATOM	2267	NH1		470	82.945	9.597	25.169	1.00 61.19
MOTA	2268	NH2		470	81.712	10.508	23.455	1.00 62.88
MOTA	2269	С	ARG	470	84.814	6.896	18.721	1.00 42.79
ATOM	2270	0	ARG	470	84.670	5.700	18.504	1.00 45.63
ATOM	2271	N	TRP	471	B4.139	7.844	18.078	1.00 41.98
ATOM	2272	CA	TRP	471	83.100	7.542	17.093	1.00 38.34
ATOM	2273	CB	TRP	471	81.844	8.307	17.451	1.00 35.68
ATOM	2274	CG	TRP	471	81.195	7.794	18.670	1.00 37.42
ATOM	2275	CD2		471	80.388	6.614	18.772	1.00 37.19
ATOM	2276	CE2		471	79.961	6.513	20.112	1.00 36.99
MOTA	2277	CE3		471	79.987	5.626	17.855	1.00 37.80
ATOM	2278	CD1		471	81.223	8.350	19.923	1.00 33.34
ATOM	2279	NEl		471	80.486	7.583	20.794	1.00 34.46
ATOM	2280	CZ2		471	79.150	5.464	20.559	1.00 38.31
MOTA	2281	CZ3		471	79.180	4.578	18.303	1.00 36.97
ATOM	2282	CH2	TRP	471	78.772	4.506	19.638	1.00 36.14

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ATOM 2283 C TRP 471 83.409 15.641 1.00 38.26 7.830 **ATOM** 2284 0 TRP 471 14.749 82.655 7.430 1.00 38.72 **ATOM** 2285 N GLU 472 84.478 8.569 15.397 1.00 37.71 ATOM 2286 CA GLU 472 84.839 8.951 14.041 1.00 38.43 **ATOM** 2287 CB GLU 472 86.014 9.924 14.087 1.00 37.56 MOTA 2288 CG GLU 472 86.146 10.835 12.871 1.00 37.26 MOTA 2289 CD GLU 472 84.930 11.728 12.625 1.00 39.02 **ATOM** 2290 OE1 GLU 472 84.361 12.301 13.571 1.00 40.26 **ATOM** 2291 OE2 GLU 472 84.568 11.879 11.445 1.00 39.35 **ATOM** 2292 C GLU 472 85.135 7.806 13.069 1.00 38.32 MOTA 2293 0 GLU 472 85.872 6.875 13.386 1.00 38.11 MOTA 2294 N LEU 473 84.535 7.884 11.883 1.00 38.44 **ATOM** 2295 - CA LEU 473 84.775 6.893 1.00 37.19 10.848 **ATOM** 2296 CB LEU 473 83.505 6.112 10.511 1.00 35.38 **ATOM** 2297 CG LEU 473 83.805 4.910 9.599 1.00 36.49 MOTA 2298 CD1 LEU 473 84.365 3.748 10.406 1.00 34.47 ATOM 2299 CD2 LEU 473 82.556 4.452 8.859 1.00 37.55 **ATOM** 2300 C LEU 473 85.283 7.623 1.00 38.21 9.601 **ATOM** 2301 0 LEU 473 84.696 8.631 9.187 1.00 38.52 ATOM 2302 N PRO 474 86.412 7.156 9.025 1.00 37.74 ATOM 2303 PRO CD 474 87.292 6.107 9.568 1.00 36.3B **ATOM** 2304 CA PRO 474 87.010 7.753 7.824 1.00 36.91 **ATOM** 2305 CB **PRO** 474 88.233 6.865 7.587 1.00 34.65 **ATOM** 2306 CG PRO 474 88.620 6.477 8.967 1.00 32.99 ATOM 2307 С PRO 474 86.036 7.663 6.660 1.00 38,15 ATOM 2308 0 PRO 474 85.536 6.578 6.362 1.00 38.24 **ATOM** 2309 N ARG 475 85.793 8.784 5.981 1.00 38.90 ATOM 2310 CA ARG 475 84.846 8.802 4.863 1.00 41.23 **ATOM** 2311 CB ARG 475 84.743 10.206 4.258 1.00 38.36 **ATOM** 2312 CG ARG 475 84.311 11.271 5.267 1.00 35.30 **ATOM** 2313 CD ARG 475 84.282 12.691 4.679 1.00 35.23 MOTA 2314 NE ARG 83.850 475 13.658 5.679 1.00 27.27 **ATOM** 2315 CZARG 475 82.585 13.859 6.011 1.00 25.77 ATOM 2316 NH1 ARG 475 81.630 13.181 5.402 1.00 25.09 ATOM 2317 NH2 ARG 82.286 14.639 475 7.047 1.00 25.24 MOTA 2318 C ARG 7.745 475 85.101 3.791 1.00 42.43 **ATOM** 2319 O ARG 475 84.160 7.212 3.204 1.00 44.06 2320 MOTA N ASP 476 86.359 7.381 3.594 1.00 44.69 ATOM 2321 CA ASP 476 86.690 6.384 2.583 1.00 48.37 MOTA 2322 CB ASP 476 88.197 6.371 2.319 1.00 52.12 **ATOM** 2323 CG ASP 476 88.988 5.925 3.521 1.00 56.56 **ATOM** 2324 OD1 ASP 476 89.299 4.718 3.613 1.00 59.72 **ATOM** 2325 OD2 ASP 476 89.294 6.779 4.376 1.00 61.19 **ATOM** 2326 C ASP 86.210 4.988 476 2.973 1.00 49.50 **ATOM** 2327 0 ASP 476 86.204 4.074 2.145 1.00 51.61 **ATOM** 2328 N ARG 477 85.852 4.814 4.241 1.00 48.26 **ATOM** 2329 CA ARG 477 85.357 3.525 4.732 1.00 47.16 ATOM 2330 CB ARG 477 85.909 3.252 6.126 1.00 49.76 **ATOM** 2331 CG ARG 477 2.723 87.325 6.088 1.00 53.26 **ATOM** 2332 CD 477 ARG 88.043 2.898 7.406 1.00 58.02 **ATOM** 2333 NE ARG 477 87.394 1.00 61.16 2.213 8.517 **ATOM** 2334 CZARG 477 87.810 2.297 9.776 1.00 63.35

SSSD/55034. V01

ATOM	2335		ARG	477	88.875	3.032	10.081	1.00 64.92
ATOM	2336		ARG	477	87.139	1.675	10.738	1.00 66.00
ATOM	2337	С	ARG	477	83.822	3.445	4.740	1.60 45.38
ATOM	2338	0	ARG	477	83.239	2.540	5.336	1.00 43.67
ATOM	2339	N	LEU	478	83.175	4.364	4.026	1.00 42.09
ATOM	2340	CA	LEU	478	81.721	4.410	3.951	1.00 37.74
ATOM	2341	CB	LEU	478	81.198	5.539	4.849	1.00 32.19
MOTA	2342	CG	LEU	478	79.673	5.638	4.973	1.00 30.21
ATOM	2343	CD1	LEU	478	79.146	4.635	5.983	1.00 22,82
ATOM	2344	CD2	LEU	478	79.313	7.035	5.422	1.00 34.82
MOTA	2345	C	LEU	478	81.329	4.702	2.514	1.00 38.75
MOTA	2346	0	LEU	478	81.818	5.669	1.935	1.00 40.60
MOTA	2347	N	VAL	479	80.477	3.863	1.925	1:00 38.78
ATOM	2348	CA	VAL	479	80.020	4.058	0.544	1.00 37.97
ATOM	2349	CB	VAL	479	80.353	2.845	-0.360	1.00 36.36
ATOM	2350	CG1	VAL	479	79.837	3.090	-1.759	1.00 33.55
ATOM	2351	CG2	VAL	479	81.868	2.626	-0.405	1.00 33.76
ATOM	2352	C	VAL	479	78.523	4.298	0.562	1.00 37.83
MOTA	2353	0	VAL	479	77.750	3.383	0.820	1.00 37.70
ATOM	2354	N	LEU	480	78.127	5.542	0.305	1.00 39.32
ATOM	2355	CA	LEU	480	76.723	5.942	0.333	1.00 38.41
ATOM	2356	CB	LEU	480	76.630	7.458	0.224	1.00 38.29
MOTA	2357	CG	LEU	480	77.287	8.226	1.377	1.00 37.99
MOTA	2358	CD1	LEU	480	77.098	9.730	1.159	1.00 34.00
MOTA	2359	CD2	LEU	480	76.666	7.785	2.703	1.00 32.79
ATOM	2360	C	LEU	480	75.893	5.287	-0.753	1.00 38.24
ATOM	2361	0	LEU	480	76.315	5.205	-1.903	1.00 39.11
ATOM	2362	N	GLY	481	74.672	4.896	-0.394	1.00 36.70
MOTA	2363	CA	GLY	481	73.811	4.223	-1.357	1.00 36.53
ATOM	2364	С	GLY	481	72.417	4.782	-1.524	1.00 37.61
ATOM	2365	0	GLY	481	72.159	5.961	-1.277	1.00 40.02
ATOM	2366	N	LYS	482	71.484	3.913	-1.911	1.00 37.52
ATOM	2367	CA	LYS	482	70.099	4.313	-2.153	1.00 39.89
MOTA	2368	CB	LYS	482	69.243	3.104	-2.551	1.00 42.44
MOTA	2369	C	LYS	482	69.447	5.028	-0.984	1.00 41.25
MOTA	2370	0	LYS	482	69.538	4.589	0.163	1.00 42.22
ATOM	2371	N	PRO	483	68.779	6.156	-1.263	1.00 41.71
MOTA	2372	CD	PRO	483	68.643	6.876	-2.537	1.00 41.01
ATOM	2373	CA	PRO	483	68.118	6.889	-0.193	1.00 42.72
ATOM	2374	CB	PRO	483	67.606	8.146	-0.906	1.00 41.26
MOTA	2375	CG	PRO	483	67.425	7.713	-2.290	1.00 40.16
ATOM	2376	С	PRO	483	66.999	6.061	0.429	1.00 44.69
MOTA	2377	0	PRO	483	66.306	5.314	-0.262	1.00 45.26
MOTA	2378	N	LEU	484	66.883	6.163	1.751	1.00 45.34
MOTA	2379	ÇA	LEU	484	65.872	5.450	2 512	1.00 47.34
MOTA	2380	CB	LEU	484	66.494	4.793	3.746	1.00 42.40
ATOM	2381	CG	LEU	484	67.517	3.668	3.535	1.00 39.50
ATOM	2382	CD1	LEU	484	68.208	3.337	4.828	1.00 33.64
ATOM	2383	CD2	LEU	484	66.861	2.419	3.003	1.00 33.44
MOTA	2384	С	LEU	484	64.733	6.391	2.927	1.00 52.14
MOTA	2385	0	LEU	484	63.611	5.941	3.142	1.00 53.64
ATOM	2386	N	GLY	485	65.013	7.697	3.025	1.00 55.25

MOTA	2387	CA	GLY	485	63.982	8.653	3.427	1.00 58.76
MOTA	2388	С	GLY	485	64.441	10.104	3.503	1.00 60.58
ATOM	2389	0	GLY	485	65.640	10.376	3.600	1.00 61.49
ATOM	2390	N	ALA	486	63.490	11.032	3.489	1.00 61.46
ATOM	2391	CA	ALA	486	63.791	12.458	3.545	1.00 63.24
MOTA	2392	CB	ALA	486	63.847	13.035	2.126	1.00 64.42
ATOM	2393	С	ALA	486	62.730	13.179	4.355	1.00 63.86
ATOM	2394	0	ALA	486	61.655	12.633	4.599	1.00 65.24
MOTA	2395	N	GLY	487	63.022	14.404	4.768	1.00 63.89
MOTA	2396	CA	GLY	487	62.054	15.158	5.538	1.00 64.30
ATOM	2397	C	GLY	487	62.431	16.617	5.623	1.00 65.34
ATOM	2398	0	GLY	487	63.071	17.154	4.718	1.00 65.98
ATOM	2399	N	ALA:	488	62.023	17.259	6.711	1.00 66.16
MOTA	2400	CA	ALA	488	62.317	18.666	6.934	1.00 66.71
MOTA	2401	CB	ALA	488	61.647	19.132	8.219	1.00 70.05
ATOM	2402	C	ALA	488	63.828	18.844	7.027	1.00 66.55
ATOM	2403	0	ALA	488	64.432	18.547	8.063	1.00 65.59
ATOM	2404	N	PHE	489	64.430	19.228	5.904	1.00 65.54
MOTA	2405	CA	PHE	489	65.875	19.457	5.807	1.00 65.40
ATOM	2406	CB	PHE	489	66.244	20.775	6.498	1.00 67.06
ATOM	2407	С	PHE	489	66.773	18.296	6.311	1.00 64.01
ATOM	2408	0	PHE	489	67.942	18.502	6.651	1.00 62.51
MOTA	2409	N	GLY	490	66.234	17.075	6.288	1.00 61.41
ATOM	2410	CA	GLY	490	66.974	15.901	6.724	1.00 55.89
MOTA	2411	С	GLY	490	66.858	14.821	5.667	1.00 53.58
ATOM	2412	0	GLY	490	65.82 5	14.703	5.000	1.00 54.22
ATOM	2413	N	GLN	491	67.899	14.006	5.543	1.00 51.23
MOTA	2414	CA	GLN	491	67.966	12.934	4.556	1.00 47.90
ATOM	2415	CB	GLN	491	68.823	13.445	3.387	1.00 50.09
ATOM	2416	CG	GLN	491	. 68.979	12.529	2.183	1.00 56.77
ATOM	2417	CD	GLN	491	69.945	13.115	1.161	1.00 60.83
ATOM	2418		GLN	491	70.283	14.292	1.218	1.00 65.11
MOTA	2419	NE2		491	70.411	12.284	0.232	1.00 63.81
ATOM	2420	C	GLN	491	68.597	11.673	5.190	1.00 45.27
ATOM	2421	0	GLN	491	69.507	11.758	6.014	1.00 45.41
ATOM	2422	N	VAL	492	68.112	10.503	4.805	1.00 41.69
ATOM	2423	CA	VAL	492	68.624	9.245	5.325	1.00 39.95
ATOM	2424	СВ	VAL	492	67.583	8.528	6.230	1.00 41.77
ATOM	2425		VAL	492	68.117	7.168	6.701	1.00 39.86
ATOM	2426		VAL	492	67.226	9.399	7.421	1.00 42.87
ATOM	2427	C	VAL	492	68.911	8.348	4.126	1.00 38.86
ATOM	2428	0	VAL	492	68.025	8.114	3.301	1.00 37.55
MOTA	2429	N	VAL	493	70.141	7.862	4.010	1.00 36.01
MOTA	2430	CA	VAL	493	70.481	6.994	2.895	1.00 37.55
ATOM	2431	СВ	VAL	493	71.471	7674	1.889	1.00 38.65
MOTA	2432		VAL	493	71.128	9.137	1.709	1.00 37.08
ATOM	2433	CG2		493	72.929	7.498	2.318	1.00 39.03
ATOM	2434	C	VAL	493	71.071	5.678	3.371	1.00 38.61
MOTA	2435	0	VAL	493	71.645	5.599	4.456	1.00 39.75
ATOM	2436	N	LEU	494	70.899	4.637	2.572	1.00 39.68
ATOM	2437	CA	LEU	494	71.460	3.345	2.910	1.00 40.98
MOTA	2438	CB	LEU	494	70.748	2.241	2.123	1.00 42.14

MOTA	2439	CG	LEU	494	71.250	0.808	2.305	1.00 40.33
ATOM	2440	CD1	LEU	494	71.186	0.425	3.765	1.00 39.62
MOTA	2441	CD2	LEU	494	70.411	-0.117	1.459	1.00 40.75
ATOM	2442	С	LEU	494	72.918	3.432	2.483	1.00 40.66
ATOM	2443	0	LEU	494	73.249	4.163	1.552	1.00 40.05
ATOM	2444	N	ALA	495	73.798	2.725	3.169	1.00 39.74
ATOM	2445	CA	ALA	495	75.202	2.768	2.820	1.00 42.06
ATOM	2446	CB	ALA	495	75.858	3.999	3.468	1.00 42.91
ATOM	2447	С	ALA	495	75.887	1.497	3.289	1.00 43.34
ATOM	2448	0	ALA	495	75.271	0.668	3.946	1.00 43.81
MOTA	2449	N	GLU	496	77.140	1.314	2.880	1.00 44.40
MOTA	2450	CA	GLU	496	77.910	0.154	3.297	1.00 45.12
MOTA	2451	CB	GLU	496	78.282	-0.722	2.106	1.00 48.62
MOTA	2452	CG	GLU	496	77.062	-1.206	1.346	1.00 56.98
MOTA	2453	CD	GLU	496	77.316	-2.476	0.567	1.00 60.32
MOTA	2454	OE1	GLU	496	76.448	-3.378	0.634	1.00 62.17
MOTA	2455	OE2	GLU	496	78.371	-2.575	-0.103	1.00 60.48
MOTA	2456	С	GLU	496	79.151	0.658	3.987	1.00 43.27
ATOM	2457	0	GLU	496	79.957	1.366	3.387	1.00 44.49
MOTA	2458	N	ALA	497	79.232	0.385	5.282	1.00 43.29
MOTA	2459	CA	ALA	497	80.374	0.799	6.086	1.00 44.01
ATOM	2460	CB	ALA	497	79.910	1.182	7.471	1.00 42.35
ATOM	2461	C	ALA	497	81.381	-0.351	6.150	1.00 45.60
ATOM	2462	0	ALA	497	80.997	-1.512	6.107	1.00 43.35
MOTA	2463	N	ILE	498	82.666	-0.025	6.206	1.00 48.78
MOTA	2464	CA	ILE	498	83.709	-1.042	6.262	1.00 49.43
MOTA	2465	CB	ILE	498	84.611	-0.977	5.014	1.00 50.66
ATOM	2466	CG2	ILE	498	85.681	-2.054	5.082	1.00 51.85
MOTA	2467	CG1	ILE	498	83.780	-1.150	3.741	1.00 50.27
MOTA	2468	CD1	ILE	498	83.073	0.112	3.255	1.00 54.24
MOTA	2469	С	ILE	498	84.572	-0.878	7.510	1.00 50.32
ATOM	2470	0	ILE	498	85.055	0.219	7.801	1.00 49.08
MOTA	2471	N	GLY	499	84.713	-1.964	8.270	1.00 51.88
ATOM	2472	CA	GLY	499	85.526	-1.958	9.480	1.00 55.86
ATOM	2473	С	GLY	499	85.061	-1.111	10.661	1.00 59.72
MOTA	2474	0	GLY	499	85.885	-0.545	11.393	1.00 61.66
MOTA	2475	N	LEU	500	83.747	-1.058	10.878	1.00 59.88
ATOM	2476	CA	LEU	500	B3.167	-0.275	11.974	1.00 58.62
ATOM	2477	CB	LEU	500	81.663	-0.556	12.086	1.00 57.41
MOTA	2478	CG	LEU	500	80.764	-0.090	10.937	1.00 55.24
ATOM	2479	CD1		500	79.331	-0.536	11.168	1.00 51.91
ATOM	2480		LEU	500	80.845	1.426	10.799	1.00 54.93
MOTA	2481	С	TEA	500	83.849	-0.565	13.306	1.00 58.51
MOTA	2482	0	LEU	500	84.226	-1.710	13.576	1.00 60.71
ATOM	2483	N	PRO	505	87.501	-6.102	10.460	1.00 82.25
MOTA	2484	CD	PRO	505	88.578	-6.722	11.248	1.00 82.69
MOTA	2485	CA	PRO	505	87.860	-4.730	10.077	1.00 80.47
MOTA	2486	CB	PRO	505	89.257	-4.557	10.686	1.00 80.88
ATOM	2487	CG	PRO	505	89.782	-5.960	10.770	1.00 81.84
ATOM	2488	С	PRO	505	87.850	-4.508	8.567	1.00 77.40
MOTA	2489	0	PRO	505	88.038	-3.391	8.087	1.00 76.83
ATOM	2490	N	ASN	506	87.632	-5.584	7.826	1.00 74.91

ATOM	2491	CA	ASN	506	87.572	-5.502	6.375	1.00 73.04
ATOM	2492	CB	asn	506	88.632	-6.406	5.749	1.00 73.39
ATOM	2493	С	asn	506	86.180	-5.938	5.929	1.00 71.75
ATOM	2494	0	ASN	506	85.918	-6.094	4.739	1.00 71.33
ATOM	2495	N	ARG	507	85.294	-6.124	6.905	1.00 69.66
ATOM	2496	CA	ARG	507	83.924	-6.534	6.638	1.00 66.59
ATOM	2497	CB	ARG	507	83.369	-7.329	7.819	1.00 69.86
MOTA	2498	C	ARG	507	83.048	-5.321	6.409	1.00 63.59
ATOM	2499	0	ARG	507	83.225	-4.291	7.070	1.00 64.09
ATOM	2500	N	VAL	508	82.126	-5.429	5.462	1.00 59.52
ATOM	2501	CA	VAL	508	81.217	-4.334	5.187	1.00 57.28
MOTA	2502	CB	VAL	508	80.905	-4.178	3.686	1.00 55.73
MOTA	2503	CG1	VAL	508	82.163	-3.952	2.922	1.00 57.01
ATOM	2504	CG2	VAL	508	80.184	-5.390	3.149	1.00 58.06
ATOM	2505	С	VAL	508	79.928	-4.614	5.935	1.00 57.10
ATOM	2506	0	VAL	508	79.483	-5.759	6.018	1.00 57.35
ATOM	2507	N	THR	509	79.345	-3.555	6.482	1.00 55.31
MOTA	2508	CA	THR	509	78.107	-3.652	7.227	1.00 50.14
ATOM	2509	CB	THR	509	78.329	-3.192	8.686	1.00 50.91
ATOM	2510	OG1		509	79.476	-3.851	9.227	1.00 49.20
ATOM	2511		THR	509	77.123	-3.524	9.559	1.00 51.96
ATOM	2512	С	THR	509	77.140	-2.705	6.528	1.00 47.53
ATOM	2513	0	THR	509	77.485	-1.558	6.242	1.GO 47.22
ATOM	2514	N	LYS	510	75.958	-3.191	6.191	1.00 45.64
ATOM	2515	CA	LYS	510	74.975	-2.333	5.551	1.00 44.44
ATOM	2516	CB	LYS	510	73.861	-3.175	4.948	1.00 46.74
ATOM	2517	CG	LYS	510	73.008	-2.420	3.950	1.00 54.51
ATOM	2518	CD	LYS	510	73.463	-2.645	2.513	1.00 54.97
ATOM	2519	CE	LYS	510	72.846	-3.917	1.934	1.00 58.25
ATOM	2520	NZ	LYS	510	73.112	-5.150	2.740	1.00 58.33
ATOM .	2521	C	LYS	510	74.430	-1.470	6.696	1.00 42.75
MOTA	2522	0	LYS	510	74.053	-2.006	7.742	1.00 43.14
ATOM	2523	N	VAL	511	74.443	-0.149	6.531	1.00 38.63
ATOM	2524	CA	VAL	511	73.975	0.757	7.576	1.00 34.16
ATOM	2525	СВ	VAL	511	75.161	1.399	8.333	1.00 35.66
ATOM	2526		VAL	511	75.922	0.340	9.100	1.00 31.46
ATOM	2527		VAL	511	76.098	2.100	7.357	1.00 35.08
ATOM ATOM	2528	C	VAL	511	73.116	1.873	7.024	1.00 31.58
ATOM	2529	0	VAL	511	72.962	1.984	5.818	1.00 33.18
ATOM	2530 2531	N Ca	ALA ALA	512	72.542	2.687	7.906	1.00 30.77
ATOM				512	71.724	3.818	7.484	1.00 28.58
ATOM	2532	CB	ALA	512	70.382	3.774	8.145	1.00 26.09
ATOM	2533	C	ALA	512	72.487	5.075	7.905	1.00 29.94
ATOM	2534	0	ALA	512	72.996	5.151	9.031	1.00 29.90
	2535 2536	N	VAL	513	72.556	6.057	7.012	1.00 28.68
ATOM ATOM		CA	VAL	513	73.286	7.290	7.280	1.00 28.26
ATOM ATOM	2537	CB	VAL	513	74.439	7.503	6.269	1.00 26.92
	2538 2539	CG1		513	75.213	8.730	6.618	1.00 25.26
ATOM		CG2		513	75.353	6.308	6.238	1.00 25.10
MOTA	2540	C	VAL	513	72.383	8.526	7.230	1.00 29.54
ATOM	2541	0	VAL	513	71.745	8.799	6.200	1.00 28.56
MOTA	2542	N	LYS	514	72.304	9.228	8.359	1.00 28.94

ATOM 2544 CB LYS 514 70.942 10.611 9.893 1.00 ATOM 2545 CG LYS 514 69.988 9.542 10.328 1.00 ATOM 2546 CD LYS 514 69.454 9.922 11.690 1.00 ATOM 2547 CE LYS 514 68.484 8.892 12.222 1.00 ATOM 2548 NZ LYS 514 67.198 8.861 11.475 1.00 ATOM 2549 C LYS 514 72.430 11.636 8.196 1.00 ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 73.425 13.487 5.693 1.00 ATOM 2555 SD MET 515 73.347 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2561 CB LEU 516 72.202 16.056 6.466 1.00 ATOM 2565 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2566 CD LEU 516 72.455 18.767 8.067 1.00 ATOM 2566 CD LEU 516 71.217 18.844 8.900 1.00 ATOM 2567 N LYS 517 66.245 18.363 2.699 1.00 ATOM 2568 CA LYS 517 66.246 18.363 2.699 1.00 ATOM 2569 CB LYS 517 66.246 18.363 2.699 1.00 ATOM 2560 CB LYS 517 66.246 18.363 2.699 1.00 ATOM 2567 N LYS 517 66.246 18.363 2.699 1.00 ATOM 2568 CA LYS 517 66.742 17.482 3.192 1.00 ATOM 2568 CB LYS 517 66.3902 17.740 1.704 1.00 ATOM 2577 CB LYS 517 66.3902 17.740 1.704 1.00 ATOM 2578 CE LYS 517 66.3902 17.740 1.704 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00	28.60 31.19 31.41 40.14 48.93 57.07 25.53 20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.98 25.32 26.60
ATOM 2544 CB LYS 514 70.942 10.611 9.893 1.00 ATOM 2545 CG LYS 514 69.988 9.542 10.328 1.00 ATOM 2546 CD LYS 514 69.454 9.922 11.690 1.00 ATOM 2547 CE LYS 514 68.484 8.892 12.222 1.00 ATOM 2548 NZ LYS 514 67.198 8.861 11.475 1.00 ATOM 2549 C LYS 514 72.430 11.636 8.196 1.00 ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 73.425 13.487 5.693 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2557 C MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2561 CB LEU 516 72.101 18.512 6.593 1.00 ATOM 2565 CG LEU 516 72.101 18.512 6.593 1.00 ATOM 2566 CD LEU 516 72.101 18.512 6.593 1.00 ATOM 2566 CD LEU 516 73.210 20.057 8.190 1.00 ATOM 2566 CD LEU 516 72.455 18.767 8.067 1.00 ATOM 2566 CD LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 CD LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 CD LEU 516 71.217 18.844 8.900 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2567 N LYS 517 66.246 18.363 2.699 1.00 ATOM 2567 N LYS 517 66.390 17.740 1.704 1.00 ATOM 2571 CD LYS 517 66.390 17.740 1.704 1.00 ATOM 2572 CE LYS 517 66.390 17.740 1.704 1.00 ATOM 2573 NZ LYS 517 66.088 17.984 2.581 1.00 ATOM 2575 N SER 518 70.520 19.455 2.507 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2578 N SER 518 70.744 19.672 1.213 1.00	31.19 31.41 40.14 48.93 57.07 25.53 20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2545 CG LYS 514 69.988 9.542 10.328 1.00 ATOM 2546 CD LYS 514 69.454 9.922 11.690 1.00 ATOM 2547 CE LYS 514 68.484 8.892 12.222 1.00 ATOM 2548 NZ LYS 514 67.198 8.861 11.475 1.00 ATOM 2549 C LYS 514 72.430 11.636 8.196 1.00 ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 72.676 13.762 7.008 1.00 ATOM 2554 CG MET 515 73.425 13.487 5.693 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2555 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2555 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2558 O MET 515 73.949 10.803 3.715 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.10 18.512 6.593 1.00 ATOM 2560 CA LEU 516 72.10 18.512 6.593 1.00 ATOM 2561 CB LEU 516 72.455 18.767 8.067 1.00 ATOM 2565 C LEU 516 71.383 17.220 6.180 1.00 ATOM 2566 CD LEU 516 71.383 17.220 6.180 1.00 ATOM 2565 C LEU 516 72.455 18.767 8.067 1.00 ATOM 2566 CD LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 69.755 18.187 2.890 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2567 N LYS 517 66.172 16.940 2.356 1.00 ATOM 2570 CG LYS 517 66.192 17.740 1.704 1.00 ATOM 2571 CD LYS 517 66.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 66.192 17.740 1.704 1.00 ATOM 2575 N SER 517 66.088 17.984 2.581 1.00 ATOM 2576 N SER 517 70.917 20.217 3.383 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2578 N SER 518 70.744 19.672 1.213 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00	31.41 40.14 48.93 57.07 25.53 20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2546 CD LYS 514 69.454 9.922 11.690 1.00 ATOM 2547 CE LYS 514 68.484 8.892 12.222 1.00 ATOM 2548 NZ LYS 514 67.198 8.861 11.475 1.00 ATOM 2549 C LYS 514 72.430 11.636 8.196 1.00 ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 72.676 13.762 7.008 1.00 ATOM 2554 CG MET 515 73.425 13.487 5.693 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2558 O MET 515 73.949 10.803 3.715 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.100 18.512 6.593 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2563 CD1 LEU 516 72.455 18.767 8.067 1.00 ATOM 2565 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 66.172 16.940 2.356 1.00 ATOM 2567 C LEU 516 71.763 16.636 3.873 1.00 ATOM 2568 CA LYS 517 66.172 16.940 2.356 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2573 NZ LYS 517 66.172 16.940 2.356 1.00 ATOM 2573 NZ LYS 517 66.088 17.984 2.581 1.00 ATOM 2575 C LYS 517 66.088 17.984 2.581 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00	40.14 48.93 57.07 25.53 20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2548 NZ LYS 514 68.484 8.892 12.222 1.00 ATOM 2548 NZ LYS 514 67.198 8.861 11.475 1.00 ATOM 2549 C LYS 514 72.430 11.636 8.196 1.00 ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 73.425 13.487 5.693 1.00 ATOM 2554 CG MET 515 72.502 13.026 4.556 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2555 CE MET 515 73.377 12.418 3.113 1.00 ATOM 2555 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2556 CE MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 71.683 14.880 6.779 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2550 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2561 CB LEU 516 72.100 18.512 6.593 1.00 ATOM 2563 CD1 LEU 516 72.110 18.512 6.593 1.00 ATOM 2564 CD2 LEU 516 73.210 20.057 8.190 1.00 ATOM 2565 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 O LEU 516 71.092 17.274 4.674 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 516 71.763 16.636 3.873 1.00 ATOM 2569 CB LYS 517 66.172 16.940 2.356 1.00 ATOM 2570 CG LYS 517 66.172 16.940 2.356 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2573 NZ LYS 517 66.172 16.940 2.356 1.00 ATOM 2574 C LYS 517 63.902 17.740 1.704 1.00 ATOM 2575 O LYS 517 66.172 16.940 2.356 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00	48.93 57.07 25.53 20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2548 NZ LYS 514 67.198 8.861 11.475 1.00 ATOM 2549 C LYS 514 72.430 11.636 8.196 1.00 ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 72.676 13.762 7.008 1.00 ATOM 2554 CG MET 515 72.676 13.762 7.008 1.00 ATOM 2555 SD MET 515 72.676 13.762 7.008 1.00 ATOM 2555 SD MET 515 72.502 13.026 4.556 1.00 ATOM 2555 CE MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2557 C MET 515 73.949 10.803 3.715 1.00 ATOM 2558 O MET 515 71.683 14.880 6.779 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2566 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 66.7432 17.182 3.192 1.00 ATOM 2561 CD LYS 517 66.7432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.72 16.940 2.356 1.00 ATOM 2572 CE LYS 517 66.902 17.740 1.704 1.00 ATOM 2573 NZ LYS 517 66.172 16.940 2.356 1.00 ATOM 2574 C LYS 517 70.917 20.217 3.383 1.00 ATOM 2575 N SER 518 70.744 19.672 1.213 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00	57.07 25.53 20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2549 C LYS 514 72.430 11.636 8.196 1.00 ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 72.676 13.762 7.008 1.00 ATOM 2554 CG MET 515 72.502 13.026 4.556 1.00 ATOM 2555 SD MET 515 73.425 13.487 5.693 1.00 ATOM 2555 CB MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.377 12.418 3.113 1.00 ATOM 2557 C MET 515 73.949 10.803 3.715 1.00 ATOM 2558 O MET 515 73.949 10.803 3.715 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2550 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.110 18.512 6.593 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2565 C LEU 516 73.210 20.057 8.190 1.00 ATOM 2566 C LEU 516 71.383 17.224 4.674 1.00 ATOM 2566 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2569 CB LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 66.172 16.940 2.356 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.917 20.217 3383 1.00 ATOM 2575 N SER 518 70.744 19.672 1.213 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00	25.53 20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2550 O LYS 514 73.544 11.714 8.722 1.00 ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 73.425 13.487 5.693 1.00 ATOM 2554 CG MET 515 72.502 13.026 4.556 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2556 CE MET 515 71.683 14.880 6.779 1.00 ATOM 2557 C MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2550 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.303 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2566 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 66.172 16.940 2.356 1.00 ATOM 2570 CG LYS 517 66.172 16.940 2.356 1.00 ATOM 2571 CD LYS 517 66.088 17.984 2.581 1.00 ATOM 2572 CE LYS 517 66.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 66.088 17.984 2.581 1.00 ATOM 2575 O LYS 517 66.088 17.984 2.581 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00	20.42 26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2551 N MET 515 71.928 12.576 7.407 1.00 ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 73.425 13.487 5.693 1.00 ATOM 2554 CG MET 515 72.502 13.026 4.556 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2557 C MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2550 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.303 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.455 18.767 8.067 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2565 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 66.172 16.940 2.356 1.00 ATOM 2570 CG LYS 517 66.172 16.940 2.356 1.00 ATOM 2571 CD LYS 517 66.088 17.984 2.581 1.00 ATOM 2572 CE LYS 517 66.902 17.740 1.704 1.00 ATOM 2573 NZ LYS 517 66.902 17.740 1.704 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 70.744 19.672 1.213 1.00	26.63 27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2552 CA MET 515 72.676 13.762 7.008 1.00 ATOM 2553 CB MET 515 73.425 13.487 5.693 1.00 ATOM 2554 CG MET 515 72.502 13.026 4.556 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2557 C MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 71.383 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 72.455 18.767 8.067 1.00 ATOM 2564 CD2 LEU 516 73.210 20.057 8.190 1.00 ATOM 2565 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 O LEU 516 71.092 17.274 4.674 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2569 CB LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 66.172 17.182 3.192 1.00 ATOM 2570 CG LYS 517 66.172 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00	27.59 28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2553 CB MET 515 73.425 13.487 5.693 1.00 ATOM 2554 CG MET 515 72.502 13.026 4.556 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2557 C MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.202 16.056 6.466 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2563 CD1 LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2569 CB LYS 517 69.755 18.187 2.890 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.088 17.984 2.581 1.00 ATOM 2572 CE LYS 517 66.088 17.984 2.581 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2576 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2577 CA SER 518 71.611 20.772 -0.809 1.00	28.22 28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2554 CG MET 515 72.502 13.026 4.556 1.00 ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.377 12.418 3.113 1.00 ATOM 2557 C MET 515 73.949 10.803 3.715 1.00 ATOM 2558 O MET 515 71.683 14.880 6.779 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 71.383 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 O LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 66.432 17.182 3.192 1.00 ATOM 2570 CG LYS 517 66.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.432 17.182 3.192 1.00 ATOM 2573 NZ LYS 517 65.088 17.984 2.581 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 71.486 20.840 0.714 1.00	28.70 32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2555 SD MET 515 73.377 12.418 3.113 1.00 ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2557 C MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 72.100 18.512 6.593 1.00 ATOM 2561 CB LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 66.172 16.940 2.356 1.00 ATOM 2570 CG LYS 517 66.072 17.984 2.581 1.00 ATOM 2571 CD LYS 517 63.902 17.740 1.704 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	32.30 24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2556 CE MET 515 73.949 10.803 3.715 1.00 ATOM 2557 C MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 71.383 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	24.88 28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2557 C MET 515 71.683 14.880 6.779 1.00 ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 71.383 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.217 18.844 8.900 1.00 ATOM 2566 O LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 70.744 19.672 1.213 1.00 ATOM 2578 CB SER 518 71.486 20.840 0.714 1.00	28.41 32.15 29.12 29.98 25.32 26.60
ATOM 2558 O MET 515 70.472 14.685 6.889 1.00 ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 71.383 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 66.172 16.940 2.356 1.00 ATOM 2571 CD LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00	32.15 29.12 29.98 25.32 26.60
ATOM 2559 N LEU 516 72.202 16.056 6.466 1.00 ATOM 2560 CA LEU 516 71.383 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2569 CB LYS 517 67.432 17.182 3.192 1.00 ATOM 2570 CG LYS 517 66.172 16.940 2.356 1.00 ATOM 2571 CD LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.486 20.840 0.714 1.00	29.12 29.98 25.32 26.60
ATOM 2560 CA LEU 516 71.383 17.220 6.180 1.00 ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2575 O LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	29.98 25.32 26.60
ATOM 2561 CB LEU 516 72.110 18.512 6.593 1.00 ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	25.32 26.60
ATOM 2562 CG LEU 516 72.455 18.767 8.067 1.00 ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	26.60
ATOM 2563 CD1 LEU 516 73.210 20.057 8.190 1.00 ATOM 2564 CD2 LEU 516 71.217 18.844 8.900 1.00 ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	
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ATOM 2565 C LEU 516 71.092 17.274 4.674 1.00 ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	22.75
ATOM 2566 O LEU 516 71.763 16.636 3.873 1.00 ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	31.50
ATOM 2567 N LYS 517 70.069 18.018 4.293 1.00 ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	32.97
ATOM 2568 CA LYS 517 69.755 18.187 2.890 1.00 ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	33.29
ATOM 2569 CB LYS 517 68.246 18.363 2.699 1.00 ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	32.20
ATOM 2570 CG LYS 517 67.432 17.182 3.192 1.00 ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	36.34
ATOM 2571 CD LYS 517 66.172 16.940 2.356 1.00 ATOM 2572 CE LYS 517 65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	43.49
ATOM 2572 CE LYS 517 .65.088 17.984 2.581 1.00 ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	53.91
ATOM 2573 NZ LYS 517 63.902 17.740 1.704 1.00 ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	58.71
ATOM 2574 C LYS 517 70.520 19.455 2.507 1.00 ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	59.37
ATOM 2575 O LYS 517 70.917 20.217 3.383 1.00 ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	31.31
ATOM 2576 N SER 518 70.744 19.672 1.213 1.00 ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	28.74
ATOM 2577 CA SER 518 71.486 20.840 0.714 1.00 ATOM 2578 CB SER 518 71.611 20.772 -0.809 1.00	32.48
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ATOM 2582 N ASP 519 69.624 22.193 1.485 1.00	35.47
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ATOM 2584 CB ASP 519 67.529 23.480 1.268 1.00	38.11
ATOM 2585 CG ASP 519 66.668 22.258 1.608 1.00	
ATOM 2586 OD1 ASP 519 67.150 21.309 2.253 1.00	41.04
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ATOM 2594 O ALA 520 71.014 24.778 5.331 1.00	41.70 49.25 34.66 33.39 33.52

ATOM	2595	N	THR	521	69.943	24.555	7.311	1.00 30.80
MOTA	2596	CA	THR	521	70.546	25.738	7.921	1.00 32.33
ATOM	2597	CB	THR	521	69.493	26.763	8.440	1.00 34.30
ATOM	2598	OG1		521	68.817	26.242	9.598	1.00 35.14
ATOM	2599	CG2	THR	521	68.484	27.109	7.366	1.00 37.70
ATOM	2600	C	THR	521	71.418	25.312	9.098	1.00 33.11
ATOM	2601	0	THR	521	71.518	24.125	9.426	1.00 31.39
ATOM	2602	N	GLU	522	72.022	26.293	9.753	1.00 34.91
ATOM	2603	CA	GLU	522	72.882	26.048	10.901	1.00 39.44
MOTA	2604	CB	GLU	522	73.516	27.357	11.360	1.00 46.96
ATOM	2605	CG	GLU	522	74.550	27.220	12.488	1.00 59.20
ATOM	2606	CD	GLU	522	75.919	26.740	12.011	1.00 64.70
ATOM	2607	OE1	GLU	522-	76.910	27.478	12.219	1.00 63.87
ATOM	2608	OE2	GLU	522	76.006	25.627	11.445	1.00 71.55
MOTA	2609	С	GLU	522	72.083	25.428	12.044	1.00 39.61
ATOM	2610	0	GLU	522	72.587	24.554	12.757	1.00 36.74
MOTA	2611	N	LYS	523	70.827	25.849	12.193	1.00 38.60
ATOM	2612	CA	LYS	523	69.970	25.327	13.252	1.00 37.77
ATOM	2613	CB	LYS	523	68.628	26.053	13.273	1.00 44.52
ATOM	2614	CG	LYS	523	67.665	25.562	14.355	1.00 51.14
ATOM	2615	CD	LYS	523	66.380	24.983	13.756	1.00 57.39
ATOM	2616	CE	LYS	523	65.499	24.376	14.852	1.00 59.17
MOTA	2617	NZ	LYS	523	64.365	23.553	14.327	1.00 62.68
ATOM	2618	С	LYS	523	69. 7 51	23.849	13.002	1.00 34.63
ATOM	2619	0	LYS	523	69.817	23.041	13.931	1.00 35.00
MOTA	2620	N	ASP	524	69.496	23.495	11.746	1.00 31.60
ATOM	2621	CA	ASP	524	69.293	22.100	11.367	1.00 29.05
MOTA	2622	CB	ASP	524	69.002	21.975	9.871	1.00 29.60
ATOM	2623	CG	ASP	524	67.695	22.626	9.472	1.00 31.90
ATOM	2624	OD1	ASP	524	66.666	22.368	10.130	1.00 38.83
MOTA	2625	OD2	ASP	524	67. 68 7	23.383	8.485	1.00 29.79
ATOM	2626	С	ASP	524	70.558	21.317	11.696	1.00 28.02
MOTA	2627	0	ASP	524	70. 4 94	20.201	12.212	1.00 28.12
ATOM	2628	N	LEU	525	71.709	21.899	11.378	1.00 28.32
ATOM	2629	CA	LEU	525	72.971	21.231	11.677	1.00 27.71
ATOM	2630	CB	LEU	525	74.173	22.085	11.257	1.00 22.53
MOTA	2631	CG	LEU	525	75.548	21.490	11.602	1.00 22.13
ATOM	2632		LEU	525	75.677	20.082	11.019	1.00 19.92
ATOM	2633		LEU	525	76.673	22.401	11.147	1.00 18.60
ATOM	2634	С	LEU	525	73.007	20.952	13.162	1.00 27.44
ATOM	2635	0	LEU	525	73.227	19.817	13.577	1.00 29.73
ATOM	2636	N	SER	526	72.689	21.976	13.947	1.00 29.09
ATOM	2637	CA	SER	526	72.672	21.891	15.412	1.00 30.83
ATOM	2638	CB	SER	526	72.222	23.230	16.006	1.00 34.25
ATOM	2639	OG	SER	526	71.966	23.147	17.397	1.00 40.67
ATOM	2640	C	SER	526	71.765	20.777	15.931	1.00 29.32
ATOM	2641	0	SER	526	72.055	20.133	16.954	1.00 28.94
MOTA	2642	N	ASP	527	70.644	20.587	15.242	1.00 26.54
MOTA	2643	CA	ASP	527	69.681	19.558	15.601	1.00 27.00
ATOM	2644	CB	ASP	527	68.392	19.798	14.829	1.00 25.91
MOTA	2645	CG	ASP	527	67.640	21.052	15.290	1.00 29.22
MOTA	2646	OD1	ASP	527	68.016	21.662	16.320	1.00 26.80

ATOM	2647	OD2	ASP	527	66.660	21.425	14.605	1.00 33.85
ATOM	2648	С	ASP	527	70.231	18.155	15.325	1.00 28.34
ATOM	2649	0	ASP	527	70.058	17.240	16.130	1.00 28.36
ATOM	2650	N	LEU	528	70.884	17.982	14.177	1.00 29.50
ATOM	2651	CA	LEU	528	71.448	16.680	13.830	1.00 30.48
ATOM	2652	CB	LEU	528	71.915	16.651	12.366	1.00 27.89
ATOM	2653	CG	LEU	528	72.443	15.305	11.832	1.00 26.48
ATOM	2654	CD1	LEU	528	71.468	14.154	12.148	1.00 21.52
ATOM	2655	CD2	LEU	528	72.722	15.383	10.333	1.00 20.23
MOTA	2656	С	LEU	528	72.583	16.308	14.804	1.00 31.69
MOTA	2657	0	LEU	528	72.688	15.145	15.222	1.00 30.09
ATOM	2658	N	ILE	529	73.397	17.298	15.195	1.00 30.79
MOTA	2659	CA	ILE	529	74.503	17.082	16.140	1.00 28.88
ATOM	2660	CB	ILE	529	75.398	18.310	16.278	1.00 25.69
ATOM	2661	CG2	ILE	529	76.541	18.007	17.217	1.00 20.54
MOTA	2662	CG1	ILE	529	75.960	18.727	14.941	1.00 23.71
ATOM	2663	CD1	ILE	529	76.981	19.831	15.035	1.00 24.21
MOTA	2664	С	ILE	529	73.951	16.767	17.533	1.00 31.52
MOTA	2665	0	ILE	529	74.439	15.850	18.213	1.00 30.66
ATOM	2666	N	SER	530	72.917	17.500	17.947	1.00 29.79
MOTA	2667	CA	SER	530	72.315	17.257	19.244	1.00 32.03
ATOM	2668	СВ	SER	530	71.176	18.239	19.492	1.00 38.91
ATOM	2669	OG	SER	530	70.266	18.231	18.412	1.00 49.86
ATOM	2670	C	SER	530	71.795	15.819	19.316	1.00 30.10
ATOM	2671	0	SER	530	71.921	15.154	20.353	1.00 31.31
ATOM	2672	N	GLU	531	71.185	15.350	18.231	1.00 27.18
MOTA	2673	CA	GLU	531	70.671	13.989	18.180	1.00 27.89
MOTA	2674	CB	GLU	531	69.923	13.744	16.881	1.00 31.29
MOTA	2675	CG	GLU	531	69.434	12.324	16.769	1.00 30.43
MOTA	2676	CD	GLU	531	68.717	12.040	15.486	1.00 30.67
MOTA	2677	OE1	GLU	531	68.293	10.892	15.317	1.00 37.79
ATOM	2678	OE2	GLU	531	68.571	12.941	14.643	1.00 34.20
ATOM	2679	С	GLU	531	71.765	12.929	18.348	1.00 26.67
MOTA	2680	0	GLU	531	71.604	11.986	19.119	1.00 24.33
MOTA	2681	N	MET	532	72.851	13.074	17.595	1.00 28.93
MOTA	2682	CA	MET	532	74.000	12.156	17.644	1.00 28.35
MOTA	2683	CB	MET	532	75.073	12.637	16.659	1.00 29.48
MOTA	2684	CG	MET	532	76.458	12.034	16.827	1.00 25.84
ATOM	2685	SD	MET	532	77.650	12.692	15.582	1.00 30.60
MOTA	2686	CE	MET	532	77.B31	14.373	16.151	1.00 20.10
MOTA	2687	C	MET	532	74.571	12.120	19.057	1.00 29.06
MOTA	2688	0	MET	532	74.876	11.053	19.589	1.00 28.22
MOTA	2689	N	GLU	533	74.640	13.289	19.688	1.00 28.61
ATOM	2690	CA	GLU	533	75.150	13.388	21.041	1.00 28.40
MOTA	2691	CB	GLU	533	75.340	14.846	21.429	1.00 29.34
ATOM	2692	CG	GLU	533	76.449	15.534	20.640	1.00 31.87
ATOM	2693	CD	GLU	533	77.822	14.923	20.892	1.00 35.10
MOTA	2694	OE1	GLU	533	78.242	14.831	22.067	1.00 37.36
MOTA	2695	OE2	GLU	533	78.490	14.543	19.913	1.00 37.71
ATOM	2696	C	GLU	533	74.211	12.684	22.023	1.00 31.03
MOTA	2697	0	GLU	533	74.651	11.936	22.906	1.00 30.76
ATOM	2698	N	MET	534	72.909	12.902	21.860	1.00 31.71

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MOTA	2699	CA	MET	534	71.940	12.256	22.727	1.00 30.58
ATOM	2700	CB	MET	534	70.510	12.620	22.315	1.00 33.53
ATOM	2701	CG	MET	534	69.538	12.624	23.509	0.50 32.45
ATOM	2702	SD	MET	534	67.778	12.682	23.150	0.50 30.95
ATOM	2703	CE	MET	534	67.523	14.422	22.895	0.50 30.50
ATOM	2704	С	MET	534	72.158	10.752	22.616	1.00 28.44
MOTA	2705	0	MET	534	72.304	10.077	23.614	1.00 27.63
ATOM	2706	N	MET	535	72.216	10.232	21.395	1.00 30.00
ATOM	2707	CA	MET	535	72.448	8.800	21.176	1.00 29.38
MOTA	2708	CB	MET	535	72.626	8.483	19.690	1.00 25.41
ATOM	2709	CG	MET	535	71.395	8.753	18.893	1.00 25.06
MOTA	2710	SD	MET	535	71.468	7.917	17.344	1.00 27.17
MOTA	2711	CE	MET	- 535	71.439	9.227	16.247	1.00 33.70
MOTA	2712	С	MET	535	73.675	8.345	21.938	1.00 30.77
ATOM	2713	0	MET	535	73.681	7.254	22.534	1.00 27.49
MOTA	2714	N	LYS	536	74.710	9.183	21.916	1.00 32.72
MOTA	2715	CA	LYS	536	75.937	8.889	22.649	1.00 34.05
ATOM	2716	CB	LYS	536	76.995	9.964	22.401	1.00 32.69
ATOM	2717	CG	LYS	536	77.719	9.838	21.073	1.00 28.00
ATOM	2718	CD	LYS	536	78.732	10.956	20.941	1.00 29.61
MOTA	2719	CE	LYS	536	79.242	11.124	19.514	1.00 26.58
MOTA	2720	NZ	LYS	536	80.020	12.389	19.460	1.00 22.22
ATOM	2721	C	LYS	536	75.652	8.769	24.145	1.00 34.80
ATOM	2722	0	LYS	536	76.004	7.763	24.750	1.00 34.44
MOTA	2723	N	MET	537	74.958	9.749	24.716	1.00 34.66
MOTA	2724	CA	MET	537	74.634	9.724	26.131	1.00 37.25
MOTA	2725	CB	MET	537	73.951	11.034	26.549	1.00 46.08
ATOM	2726	CG	MET	537	74.862	12.272	26.619	1.00 57.95
ATOM	2727	SD	MET	537	76.159	12.203	27.919	1.00 66.50
MOTA	2728	CE	MET	537	75.287	12.873	29.377	1.00 64.52
MOTA	2729	С	MET	537	73.749	8.537	26.523	1.00 36.05
MOTA	2730	0	MET	537	74.021	7.865	27.514	1.00 36.71
ATOM	2731	N	ILE	538	72.730	8.255	25.719	1.00 33.77
ATOM	2732	CA	ILE	538	71.804	7.160	26.007	1.00 30.52
MOTA	2733	CB	ILE	538	70.616	7.172	25.012	1.00 28.15
MOTA	2734	CG2	ILE	538	69.780	5.899	25.122	1.00 26.08
MOTA	2735	CG1	ILE	538	69.729	8.377	25.289	1.00 26.24
ATOM	2736	CD1		538	68.644	8.558	24.256	1.00 26.87
ATOM	2737	С	ILE	538	72.399	5.750	26.100	1.00 30.05
MOTA	2738	0	ILE	538	71.984	4.950	26.941	1.00 31.57
ATOM	2739	N	GLY	539	73.320	5.424	25.211	1.00 30.34
MOTA	2740	CA	GLY	539	73.910	4.103	25.249	1.00 28,22
ATOM	2741	С	GLY	539	73.158	3.094	24.408	1.00 31.25
ATOM	2742	0	GLY	539	72.050	3.359	23.935	1.00 32.88
MOTA	2743	N	LYS	540	73.781	1.933	24.221	1.00 31.96
ATOM	2744	CA	LYS	540	73.222	0.845	23.416	1.00 33.40
ATOM	2745	CB	LYS	540	74.342	-0.023	22.878	1.00 31.53
ATOM	2746	CG	LYS	540	75.177	0.645	21.846	1.00 37.05
MOTA	2747	CD	LYS	540	76.273	-0.266	21.361	1.00 40.15
ATOM	2748	CE	LYS	540	77.143	0.480	20.363	1.00 46.84
MOTA	2749	NZ	LYS	540	76.374	0.920	19.152	1.00 48.60
MOTA	2750	С	LYS	540	72.183	-0.090	24.023	1.00 36.22

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ATOM 2751 0 LYS 540 72.237 -0.430 25.215 1.00 40.10 **ATOM** 2752 N HIS 541 71.254 -0.521 23.175 1.00 34.86 **ATOM** 2753 HIS CA 541 70.223 -1.486 23.535 1.00 33.96 **ATOM** 2754 CB HIS 69.064 541 -0.860 24.293 1.00 31.57 MOTA 2755 CG HIS 541 68.127 -1.862 24.890 1.00 32.28 MOTA 2756 CD2 HIS 541 68.127 -2.482 26.093 1.00 32.39 ATOM 2757 ND1 HIS 67.086 541 -2.411 24.177 1.00 30.10 **ATOM** 2758 CE1 HIS 541 66.489 -3.329 24.911 1.00 33.35 MOTA 2759 NE2 HIS 541 67.096 -3.384 26.081 1.00 30.46 MOTA 2760 C HIS 541 69.720 -2.206 22.275 1.00 35.33 MOTA 2761 0 HIS 541 69.648 -1.614 21.200 1.00 34.87 **ATOM** 2762 N LYS 542 69.348 -3.478 22.430 1.00 35.42 MOTA 2763 CA LYS 542 68.908 -4.311 21.306 1.00 32.02 ATOM 2764 CB LYS 542 68.715 -5.766 21.753 1.00 30.96 MOTA 2765 C LYS 542 67.652 -3.848 20.614 1.00 30.02 ATOM 2766 0 LYS 542 67.474 -4.058 19.417 1.00 29.10 **MOTA** 2767 N ASN 543 66.778 -3.212 21.369 1.00 28.54 MOTA 2768 CA ASN 543 -2.754 65.529 20.803 1.00 28.20 MOTA 2769 CB ASN 543 64.372 -3.241 21.660 1.00 29.73 MOTA 2770 CG ASN 543 64.387 -4.739 21.840 1.00 30.74 MOTA 2771 OD1 ASN 543 64.732 -5.242 22.909 1.00 32.96 **MOTA** 2772 ND2 ASN 543 64.053 -5.462 20.787 1.00 29.58 MOTA 2773 C **ASN** 543 65.426 -1.257 20.529 1.00 28.06 MOTA 2774 0 ASN 543 64.342 -0.679 20.647 1.00 28.86 **MOTA** 2775 N ILE 544 66.546 -0.635 20.168 1.00 26.70 **ATOM** 2776 CA ILE 544 66.582 0.794 19.833 1.00 26.B1 **ATOM** 2777 CB ILE 544 67.052 1.721 21.019 1.00 24.75 MOTA 2778 CG2 ILE 544 66.338 1.353 22.306 1.00 20.02 CG1 ILE MOTA 2779 544 68.568 1.614 21.234 1.00 23.73 MOTA 2780 CD1 ILE 69.105 544 2.531 22.332 1.00 21.64 MOTA 2781 С ILE 544 67.582 0.901 18.680 1.00 27.95 MOTA 2782 0 ILE 544 68.388 -0.008 18.480 1.00 26.80 MOTA 2783 N ILE 545 67.449 1.940 1.00 29.22 17.849 MOTA 2784 CA ILE 545 68.376 2.163 16.745 1.00 27.14 MOTA 2785 CB ILE 545 67.824 3.164 15.709 1.00 26.10 MOTA 2786 CG2 ILE 545 68.920 3.556 14.731 1.00 24.70 **ATOM** 2787 CG1 ILE 545 66.625 2.568 14.955 1.00 23.78 MOTA 2788 CD1 ILE 545 66.988 1.326 14.117 1.00 22.15 **ATOM** 2789 C ILE 545 69.631 2.718 17.401 1.00 28.14 MOTA 2790 0 ILE 545 69.586 3.752 18.068 1.00 28.21 **ATOM** 2791 N ASN 546 70.740 2.011 17.221 1.00 28.40 **MOTA** 2792 CA ASN 546 72.004 2.382 17.822 1.00 28.49 **ATOM** 2793 CB ASN 546 72.709 1.122 18.345 1.00 27.05 **MOTA** 2794 CG ASN 546 71.956 0.463 19.470 1.00 27.29 MOTA 2795 OD1 ASN 546 71.793 1.031 20.540 1.00 29.92 MOTA 2796 ND2 ASN 546 71.472 -0.740 1.00 24.63 19.235 ATOM 2797 C ASN 546 72.982 3.124 16.941 1.00 28.39 ATOM 2798 0 ASN 546 73.045 2.894 15.732 1.00 29.62 **ATOM** 2799 N LEU 547 73.774 3.982 17.579 1.00 29.91 **ATOM** 2800 CA LEU 547 74.828 4.750 16.925 1.00 30.68 **ATOM** 2801 CB LEU 547 75.297 5.898 17.837 1.00 25.28 ATOM 2802 CG LEU 547 76.367 6.828 17.267 1.00 24.81

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MOTA	2803	CD1	LEU	547	75.868	7.524	15.990	1.00 22.25
ATOM	2804	CD2	LEU	547	76.716	7.853	18.313	1.00 24.17
ATOM	2805	C	LEU	547	76.016	3.812	16.629	1.00 31.67
ATOM	2806	0	LEU	547	76.481	3.090	17.509	1.00 31.34
MOTA	2807	N	LEU	548	76.475	3.823	15.380	1.00 30.60
MOTA	2808	CA	LEU	548	77.594	2.995	14.955	1.00 29.31
MOTA	2809	CB	LEU	548	77.197	2.165	13.729	1.00 25.94
ATOM	2810	CG	LEU	548	75.968	1.247	13.883	1.00 28.78
MOTA	2811	CD1	LEU	548	75.848	0.360	12.659	1.00 27.14
ATOM	2812	CD2	LEU	548	76.049	0.392	15.149	1.00 23.72
ATOM	2813	С	LEU	548	78.850	3.821	14.644	1.00 31.60
ATOM	2814	0	LEU	548	79.967	3.330	14.753	1.00 32.65
ATOM	2815	N	GLY	549	78.665	5.076	14.248	1.00 32.22
MOTA	2816	CA	GLY	549	79.795	5.928	13.937	1.00 31.40
ATOM	2817	C	GLY	549	79.344	7.267	13.391	1.00 30.78
MOTA	2818	0	GLY	549	78.140	7.536	13.291	1.00 29.84
ATOM	2819	N	ALA	550	80.320	8.099	13.045	1.00 31.88
ATOM	2820	CA	ALA	550	80.073	9.416	12.485	1.00 30.14
ATOM	2821	CB	ALA	550	79.634	10.382	13.590	1.00 31.08
ATOM	2822	С	ALA	550	81.291	9.978	11.742	1.00 28.78
MOTA	2823	0	ALA	550	82.447	9.705	12.102	1.00 26.39
MOTA	2824	N	CYS	551	81.011	10.690	10.651	1.00 28.48
MOTA	2825	CA	CYS	551	82.012	11.391	9.846	1.00 23.69
ATOM	2826	CB	CYS	551	81.825	11.128	8.352	1.00 24.18
ATOM	2827	SG	CYS	551	81.870	9.395	7.840	1.00 28.40
ATOM	2828	С	CYS	551	81.612	12.847	10.127	1.00 20.99
ATOM	2829	0	CYS	551	80.561	13.282	9.684	1.00 22.11
ATOM	2830	N	THR	552	82.357	13.524	10.996	1.00 20.18
ATOM	2831	CA	THR	552	82.073	14.914	11.349	1.00 22.79
ATOM	2832	CB	THR	552	82.090	15.080	12.874	1.00 23.16
ATOM	2833	OG1	THR	552	83.408	14.803	13.363	1.00 23.52
ATOM	2834	CG2	THR	552	81.125	14.112	13.529	1.00 25.31
ATOM	2835	C	THR	552	83.138	15.886	10.824	1.00 24.74
MOTA	2836	0	THR	552	82.939	17.103	10.782	1.00 22.75
MOTA	2837	N	GLN	553	84.276	15.334	10.431	1.00 26.82
ATOM	2838	CA	GLN	553	85.387	16.153	9.980	1.00 26.99
ATOM	2839	CB	GLN	553	B6.686	15.627	10.602	1.00 26.40
MOTA	2840	CG	GLN	553	86.632	15.494	12.141	1.00 22.69
ATOM	2841	CD	GLN	553	86.438	16.836	12.823	1.00 25.90
ATOM	2842		GLN	553	87.259	17.729	12.656	1.00 29.03
ATOM	2843	NE2		553	85.351	16.994	13.566	1.00 23.53
MOTA	2844	C	GLN	5 53	85.502	16.216	8.466	1.00 26.23
ATOM	2845 2846	0	GLN	553	85.177	15.259	7.779	1.00 30.00
		N	ASP	554	85.863	17.394	7.968	1.00 26.54
ATOM	2847 2848	CA	ASP	55 4	86.084	17.631	6.531	1.00 28.38
ATOM ATOM	2849	.CB	ASP	55 4	87.410	17.031	6.105	1.00 26.78
ATOM		CG	ASP	554 554	88.538	17.570	6.912	1.00 31.53
ATOM	2850 2851	OD1		554 554	88.789	18.795	6.823	1.00 35.18
		OD2		554 554	89.141	16.795	7.665	1.00 29.04
ATOM	2852	C	ASP	554 554	85.011	17.221	5.545	1.00 29.14
ATOM	2853	0	ASP	554	85.278	16.468	4.610	1.00 31.22
ATOM	2854	N	GLY	555	83.824	17.793	5.709	1.00 31.20

MOTA	2855	CA	GLY	555	82.723	17.490	4.811	1.00 28.83
ATOM	2856	С	GLY	555	81.446	17.413	5.602	1.00 24.84
MOTA	2857	0	GLY	555	81.448	17.647	6.814	1.00 21.78
ATOM	2858	N	PRO	556	80.317	17.093	4.953	1.00 24.29
MOTA	2859	CD	PRO	556	80.213	16.783	3.510	1.00 19.37
MOTA	2860	CA	PRO	556	79.010	16.973	5.615	1.00 25.11
MOTA	2861	CB	PRO	556	78.107	16.497	4.477	1.00 22.88
MOTA	2862	CG	PRO	556	79.077	15.832	3.485	1.00 23.50
ATOM	2863	C	PRO	556	79.006	15.982	6.777	1.00 27.67
ATOM	2864	0	PRO	556	79.676	14.947	6.736	1.00 27.13
MOTA	2865	N	LEU	557	78.253	16.297	7.820	1.00 29.27
MOTA	2866	CA	LEU	557	78.164	15.405	8.972	1.00 31.19
MOTA	2867		LEU	557	77.583	16.130	10.188	1.00 29.94
ATOM	2868	CG	LEU	557	77.019	15.260	11.323	1.00 26.87
ATOM	2869	CD1	LEU	557	78.131	14.540	12.062	1.00 23.83
MOTA	2870		LEU	557	76.237	16.146	12.275	1.00 23.80
ATOM	2871	C	LEU	557	77.291	14.193	8.651	1.00 31.97
MOTA	2872	0	LEU	557	76.158	14.332	8.184	1.00 31.18
MOTA	2873	N	TYR	558	77.857	13.010	8.882	1.00 31.12
ATOM	2874	CA	TYR	558	77.145	11.767	8.664	1.00 28.86
MOTA	2875	СВ	TYR	558	77.905	10.869	7.694	1.00 28.58
ATOM	2876	CG	TYR	558	78.017	11.395	6.281	1.00 32.33
ATOM	2877		TYR	558	79.034	10.962	5.443	1.00 35.23
MOTA	2878		TYR	558	79.161	11.447	4.151	1.00 37.54
ATOM	2879		TYR	558	77.123	12.336	5.787	1.00 35.27
ATOM	2880	CE2	TYR	558	77.248	12.832	4.493	1.00 36.43
MOTA	2881	CZ	TYR	558	78.276	12.382	3.680	1.00 37.05
ATOM	2882	OH	TYR	558	78.423	12.869	2.394	1.00 39.97
ATOM	2883	C	TYR	558	77.000	11.071	10.004	1.00 26.63
ATOM	2884	0	TYR	558	77.985	10.885	10.725	1.00 24.67
ATOM ATOM	2885	N	VAL	559	75.756	10.774	10.365	1.00 28.15
ATOM	2886	CA	VAL	559	75.429	10.070	11.610	1.00 27.70
ATOM	2887	CB CG1	VAL	559	74.262	10.770	12.372	1.00 26.63
ATOM	2888 2889	CG2		559 550	73.876	9.959	13.603	1.00 24.70
ATOM	2890	CG2	VAL	559 559	74.673	12.186	12.792	1.00 26.71
ATOM	2891	0	VAL	559	75.061 73.965	8.635 8.357	11.205	1.00 27.08
MOTA	2892	N	ILE	560	76.002	7.729	10.710	1.00 25.39
ATOM	2893	CA	ILE	560	75.820	6.335	11.399	1.00 28.25
ATOM	2894	CB	ILE	560	77.225	5.682	11.000 10.678	1.00 29.62 1.00 30.06
ATOM	2895	CG2		560	77.045	4.279		
ATOM	2896	CG1		560	78.004	6.557	10.101 9.686	1.00 31.58
ATOM	2897	CD1		560	79.492	6.239	9.629	1.00 27.50 1.00 23.31
ATOM	2898	C	ILE	560	75.472	5.488	12.032	1.00 23.31
ATOM	2899	0	ILE	560	75.586	5.234	13.130	
ATOM	2900	N	VAL	561	73.857	5.078	11.687	1.00 27.32 1.00 29.09
ATOM	2901	CA	VAL	561	73.053	4.228	12.568	1.00 29.09
ATOM	2902	СВ	VAL	561	71.743	4.932	13.037	1.00 28.70
ATOM	2903	CG1		561	72.072	6.139	13.872	1.00 23.29
ATOM	2904	CG2		561	70.887	5.312	11.870	1.00 22.31
ATOM	2905	C	VAL	561	72.731	2.848	11.870	1.00 22.38
ATOM	2906	0	VAL	561	73.052	2.590	10.783	1.00 27.88
	2200	-	72.23		. 3 . 032	2.330	10.703	1.00 27.88

MOTA	2907	N	GLU	562	72.143	1.969	12.754	1.00 27.38	
MOTA	2908	CA	GLU	562	71.759	0.616	12.347	1.00 28.01	
MOTA	2909	CB	GLU	562	71.246	-0.161	13.555	1.00 25.37	
MOTA	2910	CG	GLU	562	72.322	-0.487	14.570	1.00 29.22	
ATOM	2911	CD	GLU	562	71.785.	-1.190	15.796	1.00 30.94	
ATOM	2912	OE1	GLU	562	72.440	-2.135	16.271	1.00 34.82	
ATOM	2913	OE2	GLU	562	70.716	-0.795	16.297	1.00 32.77	
ATOM	2914	С	GLU	562	70.695	0.610	11.266	1.00 29.83	
MOTA	2915	0	GLU	562	69.822	1.452	11.274	1.00 34.69	
ATOM	2916	N	TYR	563	70.755	-0.364	10.362	1.00 31.35	
ATOM	2917	CA	TYR	563	69.806	-0.527	9.255	1.00 33.79	
ATOM	2918	CB	TYR	563	70.586	-0.987	8.022	1.00 32.37	
ATOM -	2919	CG	TYR ·	- 563	69.759	-1.232	6.778	1.00 31.70	
ATOM	2920	CD1	TYR	563	68.858	-0.277	6.319	1.00 35.00	
ATOM	2921	CE1	TYR	563	68.101	-0.490	5.161	1.00 35.62	
ATOM	2922	CD2	TYR	563	69.888	-2.416	6.053	1.00 31.64	
ATOM	2923	CE2	TYR	563	69.138	-2.644	4.894	1.00 32.36	
ATOM	2924	CZ	TYR	563	68.242	-1.674	4.462	1.00 36.20	
ATOM	2925	OH	TYR	563	67.494	-1.906	3.340	1.00 39.54	
ATOM	2926	C	TYR	563	68.668	-1.527	9.593	1.00 37.26	
MOTA	2927	0	TYR	563	68.915	-2.566	10.212	1.00 38.86	
ATOM	2928	N	ALA	564	67.428	-1.180	9.220	1.00 39.09	
ATOM	2929	CA	ALA	564	66.256	-2.027	9.467	1.00 37.64	
ATOM	2930	CB	ALA	564	65.290	-1.317	10.366	1.00 41.34	
ATOM	2931	C	ALA	564	65.600	-2.337	8.124	1.00 39.33	
ATOM	2932	0	ALA	564	64.700	-1.628	7.661	1.00 41.28	
MOTA	2933	N	SER	565	66.033	-3.432	7.515	1.00 40.21	
ATOM	2934	CA	SER	565	65.567	-3.867	6.202	1.00 40.22	
MOTA	2935	CB	SER	565	66.302	-5.133	5.808	1.00 38.50	
ATOM	2936	OG	SER	565	66.174	-6.084	6.847	1.00 37.66	
MOTA	2937	C	SER	565	64.095	-4.087	5.987	1.00 42.30	
ATOM	2938	0	SER	565	63.657	-4.155	4.840	1.00 46.83	
ATOM	2939	N	LYS	566	63.322	-4.248	7.054	1.00 42.84	
MOTA	2940	CA	LYS	566	61.893	-4.462	6.883	1.00 41.84	
MOTA	2941	CB	LYS	566	61.455	-5.681	7.684	1.00 44.88	
MOTA	2942	CG	LYS	566	62.003	-6.977	7.088	1.00 48.86	
ATOM	2943	CD	LYS	566	61.929	-8.148	8.040	1.00 51.41	
ATOM	2944	CE	LYS	566	62.582	-9.362	7.426	1.00 53.89	
ATOM	2945	NZ	LYS	566	62.706		8.417	1.00 59.37	
ATOM ATOM	2946	C	LYS	566	61.029	-3.234	7.143	1.00 41.89	
ATOM	2947 2948	0	LYS	566	59.815	-3.337	7.341	1.00 43.68	
ATOM	2949	N CA	GLY GLY	567	61.663	-2.061	7.100	1.00 39.50	
ATOM	2950	CA	GLY	567	60.956	-0.808	7.291	1.00 36.69	
ATOM				567	60.306	-0.640	8.644	1.00 35.86	
ATOM	2951 2952	o N	GLY ASN	567 560	60.727	-1.265	9.614	1.00 35.90	
ATOM	2953	CA	asn	568 569	59.296	0.218	8.711	1.00 35.45	
ATOM	2954			568 560	58.615	0.447	9.966	1.00 38.10	
		CB CG	ASN	568	57.961	1.839	10.029	1.00 40.77	
MOTA MOTA	2955 2956		ASN	568 560	56.701	1.962	9.163	1.00 43.52	
ATOM		OD1		568 569	55.718	1.241	9.338	1.00 44.01	
ATOM	2957	ND2		568	56.710	2.932	8.263	1.00 45.39	
ALON	2958	С	ASN	568	57.610	-0.657	10.269	1.00 38.91	

ATOM 2959 O **ASN** 56B 57.218 -1.420 9.384 1.00 39.95 **ATOM** 2960 N LEU 569 57.204 -0.717 11.534 1.00 38.93 **ATOM** 2961 CA LEU 569 56.256 -1.692 12.047 1.00 36.49 MOTA 2962 CB LEU -1.507 569 56.126 13.555 1.00 36.53 **ATOM** 2963 CG LEU 569 55.150 -2.417 1.00 35.27 14.290 **ATOM** 2964 CD1 LEU 569 55.550 -3.865 14.047 1.00 31.86 **ATOM** 2965 CD2 LEU 569 55.148 -2.067 15.768 1.00 35.00 **ATOM** 2966 C LEU 569 54.875 -1.622 11.391 1.00 37.19 **ATOM** 2967 LEU 0 569 54.231 -2.654 11.175 1.00 38.40 **ATOM** 2968 N ARG 570 54.386 -0.420 11.101 1.00 36.63 MOTA 2969 CA ARG 570 53.068 -0.294 10.485 1.00 36.68 MOTA 2970 CB ARG 570 52.739 1.168 10.188 1.00 37.76 **ATOM** 2971 CG ~ ARG 570 51.339 1.361 9.623 1.00 46.41 **ATOM** 2972 CD **ARG** 570 51.210 2.680 8.889 1.00 56.33 **ATOM** 2973 NE **ARG** 570 52.162 2.785 7.779 1.00 63.05 **ATOM** 2974 CZ**ARG** 570 53.010 3.798 7.603 1.00 66.33 MOTA 2975 NH1 ARG 570 53.032 4.809 8.468 1.00 65.15 MOTA 2976 NH2 ARG 570 53.853 3.786 6.580 1.00 66.56 **ATOM** 2977 С ARG 570 53.046 -1.094 9.193 1.00 35.55 **ATOM** 2978 0 ARG 570 52.248 -2.015 9.018 1.00 35.33 MOTA 2979 GLU N 571 53.978 -0.758 8.320 1.00 37.20 MOTA 2980 CA GLU 571 54.128 -1.401 7.030 1.00 38.32 MOTA 2981 CB GLU 571 55.247 -0.695 6.261 1.00 40.15 MOTA 2982 CG GLU 571 55.001 0.803 6.152 1.00 49.09 MOTA 2983 CD GLU 571 56.118 1.557 5.442 1.00 58.16 ATOM 2984 OE1 GLU 571 57.279 1.073 5.421 1.00 61.41 MOTA 2985 OE2 GLU 571 55.824 2.660 4.914 1.00 61.27 **ATOM** 2986 С GLU 571 54.406 -2.906 7.170 1.00 36.74 ATOM 2987 GLU 0 571 53.863 -3.721 6.410 1.00 35.74 **ATOM** 2988 TYR 572 N 55.241 -3.266 8.141 1.00 35.13 MOTA 2989 CA TYR 572 55.591 -4.665 8.401 1.00 37.12 ATOM 2990 CB TYR 572 56.591 -4.736 9.560 1.00 34.39 ATOM 2991 CG TYR 572 56.984 -6.128 10.029 1.00 33.48 MOTA 2992 CD1 TYR 572 57.980 -6.869 9.367 1.00 29.76 MOTA 2993 CE1 TYR 572 58.394 -8.119 9.845 1.00 27.14 **ATOM** 2994 CD2 TYR 572 56.406 -6.681 11.183 1.00 32.40 **MOTA** 2995 CE2 TYR 572 56.814 -7.931 11.669 1.00 30.83 MOTA 2996 CZ TYR 572 57.807 -8.641 10.995 1.00 33.73 **MOTA** 2997 OH TYR 572 58.201 -9.872 11.480 1.00 37.16 **ATOM** 2998 C TYR 572 54.330 -5.468 8.729 1.00 38.92 MOTA 2999 0 TYR 572 54.108 -6.553 8.183 1.00 39.22 **ATOM** 3000 N LEU 573 53.507 -4.922 9.618 1.00 38.41 **ATOM** 3001 CA LEU 573 52.261 -5.563 10.016 1.00 37.56 3002 CB ATOM LEU 573 51.573 -4.711 11.084 1.00 36.44 **ATOM** 3003 CG LEU 573 52.270 -4.617 12.437 1.00 33.91 **ATOM** 3004 CD1 LEU 573 51.555 -3.626 13.372 1.00 31.60 -6.024 ATOM 3005 CD2 LEU 573 52.313 13.003 1.00 30.78 MOTA 3006 C LEU 573 51.315 -5.738 8.826 1.00 37.51 MOTA 3007 0 LEU 573 50.847 -6.836 8.539 1.00 36.70 **ATOM** 3008 N GLN 574 51.045 -4.643 8.125 1.00 40.10 MOTA 3009 CA GLN 574 50.141 -4.678 6.986 1.00 41.10 MOTA 3010 CB 49.938 -3.272 GLN 574 6.439 1.00 40.12

ATOM	3011	CG	GLN	574	49.171	-2.381	7.374	1.00 40.77
ATOM	3012	CD	GLN	574	49.079	-0.987	6.852	1.00 43.90
ATOM	3013	OE1	GLN	574	49.679	-0.652	5.835	1.00 46.93
ATOM	3014	NE2	GLN	574	48.357	-0.143	7.558	1.00 46.85
ATOM	3015	С	GLN	574	50.546	-5.638	5.875	1.00 41.31
MOTA	3016	0	GLN	574	49.699	-6.323	5.309	1.00 44.33
MOTA	3017	N	ALA	575	51.840	-5.735	5.601	1.00 41.46
ATOM	3018	CA	ALA	575	52.317	-6.628	4.555	1.00 39.80
ATOM	3019	CB	ALA	575	53.745	-6.301	4.218	1.00 40.58
MOTA	3020	С	ALA	575	52.197	-8.096	4.947	1.00 40.86
ATOM	3021	0	ALA	575	52.527	-8.975	4.165	1.00 41.50
ATOM	3022	N	ARG	576	51.757	-8.359	6.168	1.00 42.47
ATOM	3023	CA ·	· ARG ·	-576	-51.624	-9. 7 26	6.641	1.00 42.68
MOTA	3024	CB	ARG	576	52.679	-9.988	7.716	1.00 41.04
MOTA	3025	CG	ARG	576	54.095	-9.958	7.161	1.00 42.73
ATOM	3026	\mathbf{c}	ARG	576	55.156	-9.943	8.257	1.00 45.59
ATOM	3027	NE	ARG	576	56.514	-9.870	7.695	1.00 43.89
ATOM	3028	CZ	ARG	576	56.981	-8.856	6.969	1.00 43.35
MOTA	3029	NH1	ARG	576	56.219	-7.803	6.703	1.00 44.85
MOTA	3030	NH2	ARG	576	58.215	-8.902	6.497	1.00 41.84
ATOM	3031	C	ARG	576	50.232	-10.014	7.180	1.00 44.86
MOTA	3032	0	ARG	576	50.043	-10.943	7.970	1.00 46.08
ATOM	3033	N	ARG	577	49.258	-9.216	6.753	1.00 46.72
MOTA	3034	C'A	ARG	577	47.877	-9.401	7.196	1.00 47.61
ATOM	3035	CB	ARG	577	46.994	-8.239	6.723	1.00 46.35
ATOM	3036	CG	ARG	577	47.101	-6.995	7.581	1.00 47.71
ATOM	3037	CD	ARG	5 77	46.329	-5.831	6.999	1.00 49.15
MOTA	3038	NE	ARG	577	46.213	-4.735	7.957	1.00 53.23
ATOM	3039	CZ	ARG	577	45.584	-3.587	7.725	1.00 54.38
ATOM	3040	NH1	ARG	577 .	45.020	-3.368	6.549	1.00 56.41
ATOM	3041	NH2		577	45.481	-2.676	8.686	1.00 58.13
ATOM	3042	С	ARG	577	47.298	-10.740	6.743	1.00 47.36
ATOM	3043	0	ARG	577		-11.031	5.550	1.00 48.52
ATOM	3044	N	GLN	594	53.349	-13.948	7.960	1.00 68.05
ATOM	3045	CA	GLN	594		-14.067	8. 7 72	1.00 66.75
ATOM	3046	CB	GLN	594		-15.220	8.277	1.00 66.87
MOTA	3047	С	GLN	594		-14.284	10.233	1.00 64.71
ATOM	3048	C	GLN	594		-15.264	10.580	1.00 64.86
MOTA	3049	N	LEU	595		-13.335	11.074	1.00 61.14
ATOM	3050	CA	TEA	595		-13.422	12.480	1.00 58.19
ATOM	3051	CB	LEU	395		-12.008	13.056	1.00 56.33
ATOM	3052	CG	LEU	595		-11.147	12.203	1.00 57.36
ATOM	3053	CD1		595	53.375	-9.692	12.533	1.00 59.51
ATOM	3054	CD2		595		-11.598	12.382	1.00 56.98
ATOM	3055	C	LEU	595		-14.237	13.251	1.00 56.25
MOTA		0	LEU	595		-14.359	12.834	1.00 56.60
MOTA	3057	N	SER	596		-14.845	14.341	1.00 53.07
ATOM	3058	CA	SER	596		-15.642	15.229	1.00 48.64
ATOM	3059	CB	SER	596		-16.841	15.736	1.00 46.41
ATOM	3060	OG	SER	596		-16.435	16.737	1.00 46.50
ATOM	3061	С	SER	596		-14.756	16.423	1.00 48.95
ATOM	3062	0	SER	596	51.492	-13.767	16.649	1.00 49.39

ATOM	3063	N	SER	597	49.833 -15	.163	17.242	1.00	50.27
MOTA	3064	CA	SER	597	49.469 -14	.387	18.424	1.00	51.93
MOTA	3065	CB	SER	597	48.391 -15	.123	19.225	1.00	52.03
MOTA	3066	OG	SER	597	47.540 -15	. 854	18.365	1.00	52.95
ATOM	3067	С	SER	597	50.685 -14	.143	19.314	1.00	52.72
ATOM	3068	0	SER	597	50.792 -13	.093	19.943	1.00	55.04
MOTA	3069	N	LYS	598	51.613 -15	.100	19.344	1.00	53.55
ATOM	3070	CA	LYS	598	52.824 -14	. 961	20.159	1.00	53.84
ATOM	3071	CB	LYS	598	53.566 -16	. 295	20.248	1.00	54.25
ATOM	3072	CG	LYS	598	54.376 -16	.457	21.524	1.00	57.30
ATOM	3073	CD	LYS	598	55.057 -17	.824	21.570	1.00	58.11
MOTA	3074	CE	LYS	598	55.780 -18	.055	22.893		59.00
MOTA	3075	NZ	LYS	598	54.840 -18	.169	24.043		57.85
MOTA	3076	С	LYS	598	53.728 -13	. 909	19.527		52.48
MOTA	3077	0	LYS	598	54.273 -13	. 052	20.227	1.00	51.72
MOTA	3078	N	ASP	599	53.842 -13	. 960	18.198		50.65
ATOM	3079	CA	ASP	599	54.657 -13	.021	17.435		48.52
ATOM	3080	CB	ASP	599	54.568 -13	. 294	15.929	1.00	46.71
MOTA	3081	CG	ASP	599	55.233 -14	.607	15.515	1.00	48.88
ATOM	3082	OD1	ASP	599	55.898 -15	.260	16.344	1.00	53.76
MOTA	3083	OD2	ASP	599	55.100 -14	. 986	14.330	1.00	46.70
ATOM	3084	C	ASP	599	54.173 -11	. 598	17.706	1.00	48.66
MOTA	3085	0	ASP	599	54.976 -10	. 703	17.960	1.00	52.86
ATOM	3086	N	LEU	600	52.852 -11	.406	17.684	1.00	44.53
ATOM	3087	CA	LEU	600	52.272 -10	.099	17.938	1.00	41.06
ATOM	3088	CB	LEU	600	50.774 ~10	.100	17.632	1.00	39.23
ATOM	3089	CG	LEU	600	50.354 -10	.374	16.178	1.00	36.50
ATOM	3090	CD1	LEU	600	48.850 -10	. 272	16.063	1.00	34.99
MOTA	3091	CD2	LEU	600	51.000 -9	. 393	15.232	1.00	33.72
ATOM	3092	C	LEU	600	52.543 -9	.633	19.369	1.00	40.96
ATOM	3093	0	LEU	600	52.890 -8	.467	19.580	1.00	42.04
MOTA	3094	N	VAL	601	52.417 -10	. 533	20.348	1.00	41.02
ATOM	3095	CA	VAL	601	52.685 -10	.156	21.744	1.00	43.57
ATOM	3096	CB	VAL	601	52.236 -11.	.229	22.791	1.00	43.60
ATOM	3097	CG1	VAL	601	52.254 -10.	.607	24.205	1.00	43.44
MOTA	3098		VAL	601	50.848 -11.	. 761	22.464	1.00	42.33
ATOM	3099	С	VAL	601	54.192 -9.	. 904	21.901	1.00	42.85
MOTA	3100	0	VAL	601	54.611 -8	. 989	22.611	1.00	44.28
ATOM	3101	N	SER	602	54.986 ~10.	.685	21.175	1.00	41.33
ATOM	3102	CA	SER	602	56.442 -10.	. 581	21.180	1.00	41.43
ATOM	3103	CB	SER	602	57.014 -11.	. 64 B	20.245	1.00	40.94
ATOM	3104	OG	SER	602	58.434 -11.	.612	20.184	1.00	46.26
ATOM	3105	C	SER	602	56.859 -9.	.176	20.722	1.00	40.58
ATOM	3106	0	SER	602	57.629 -8.	.497	21.403	1.00	42.32
MOTA	3107	N	CYS	603	56.318 -8.	. 73 7	19.589	1.00	38.34
MOTA	3108	CA	CYS	603	56.580 -7.	.409	19.051	1.00	37.28
MOTA	3109	CB	CYS	603	55.715 -7.	.170	17.815	1.00	38.09
ATOM	3110	SG	CYS	603	55.735 -5.	.497	17.170	0.50	42.18
MOTA	3111	C	CYS	603	56.282 -6.	. 337	20.105	1.00	35.81
MOTA	3112	0	CYS	603	57.038 -5.	.380	20.241	1.00	37.87
MOTA	3113	N	ALA	604	55.198 -6.	.508	20.858	1.00	33.96
ATOM	3114	CA	ALA	604	54.804 -5.	. 572	21.911	1.00	34.97

439

ATOM 1.00 34.13 3115 CB ALA 604 53.393 -5.917 22.409 **ATOM** 3116 C 604 ALA 55.791 -5.610 23.081 1.00 36.68 MOTA 3117 0 ALA 604 56.085 -4.585 23.704 1.00 36.78 ATOM 3118 N TYR 605 56.281 -6.807 23.385 1.00 37.68 MOTA 3119 CA TYR 605 57.254 -7.005 24.461 1.00 38.38 MOTA 3120 CB TYR 605 -8.498 57.533 24.643 1.00 37,62 **ATOM** 3121 CG TYR 605 -8.806 58.635 25.622 1.00 36.56 ATOM CD1 TYR 3122 605 -8.509 58.498 26.974 1.00 39.05 MOTA 3123 CE1 TYR 605 59.520 -8.809 27.893 1.00 41.37 ATOM 3124 CD2 TYR 605 59.812 -9.407 25.198 1.00 38.09 MOTA 3125 CE2 TYR -9.711 605 60.848 26.105 1.00 38.55 **ATOM** 3126 CZTYR 605 60.692 -9.409 27.454 1.00 40.73 - ATOM 3127 OH TYR 605 -9.704 61.707 28.348 1.00 41.44 **ATOM** 3128 С TYR 605 58.549 -6.267 24.123 1.00 38.44 **ATOM** 3129 o TYR 605 59.053 -5.485 24.937 1.00 40.78 ATOM 3130 N GLN 606 59.053 -6.501 22.908 1.00 36.07 ATOM 3131 CA GLN 606 60.276 -5.872 22.398 1.00 35,28 MOTA 3132 CB GLN 606 60.594 -6.415 21.002 1.00 34.24 **ATOM** 3133 CG GLN 606 61.105 -7.851 21.005 1.00 32.26 ATOM 3134 CD GLN 606 61.339 -8.388 19.608 1.00 30.17 **ATOM** 3135 OE1 GLN 606 62.274 -7.988 18.907 1.00 31.89 ATOM 3136 NE2 GLN 606 60.471 -9.285 19.182 1.00 30.68 MOTA 3137 C GLN 606 60.210 -4.335 22.355 1.00 36.39 MOTA 3138 0 GLN 606 61.206 -3.660 22.632 1.00 39.59 MOTA 3139 N VAL 607 59.040 -3.798 22.006 1.00 32.78 MOTA 3140 CA VAL 607 58.839 -2.350 21.944 1.00 30.29 MOTA 3141 CB VAL 607 57.489 -1.982 21.221 1.00 28.48 ATOM 3142 CG1 VAL 607 57.219 -0.488 21.298 1.00 28.68 MOTA 3143 CG2 VAL 607 57.535 -2.416 19.742 1.00 22.96 ATOM 3144 С VAL 58.868 -1.766 607 23.364 1.00 30.21 **ATOM** 3145 0 VAL 607 59.469 -0.705 23.591 1.00 31.24 **ATOM** 3146 N ALA 608 58.224 -2.451 24.311 1.00 27.88 **MOTA** 3147 CA ALA 608 58.187 -2.001 25.694 1.00 27.66 **ATOM** 3148 CB ALA -2.874 608 57.242 26.494 1.00 26.42 **MOTA** 3149 C ALA 608 59.585 -2.019 26.309 1.00 29.04 MOTA 3150 0 ALA 608 59.950 -1.144 27.094 1.00 27.53 **ATOM** 3151 N ARG 609 60.377 -3.013 25.932 1.00 28.91 **ATOM** 3152 CA ARG 609 61.733 -3.120 26.440 1.00 31.64 **ATOM** 3153 CB ARG 609 62.394 -4.405 25.953 1.00 33.78 **ATOM** 3154 CG ARG 609 61.672 -5.647 26.373 1.00 38.53 **ATOM** 3155 CD **ARG** 609 62.636 -6.791 26.448 1.00 41.78 **ATOM** 3156 NE ARG 609 63.319 -6.83B 27.733 1.00 47.58 MOTA 3157 CZARG 609 64.441 -7.510 27.955 1.00 51.52 ATOM 3158 NH1 ARG 609 65.012 -8.179 26.964 1.00 50.61 MOTA 3159 NH2 ARG 64.954 609 -7.569 29.186 1.00 54.36 **ATOM** 3160 C ARG 62.581 609 -1.918 26.024 1.00 33.26 **ATOM** 3161 0 ARG 609 63.144 -1.221 26.885 1.00 34.50 **ATOM** 3162 N GLY 610 62.624 -1.650 24.717 1.00 30.25 MOTA 3163 CA GLY 610 63.395 -0.534 24.199 1.00 25.40 MOTA 3164 C GLY 610 63.010 0.730 24.930 1.00 24.12 **ATOM** 3165 0 GLY 610 63.857 1.507 25.345 1.00 24.74 **ATOM** 3166 N MET 611 61.712 0.907 25.131 1.00 25.81

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1	ATOM	3167	CA	MET	611	61.192	2.062	25.843	1.00 26.95
7	ATOM	3168	CB	MET	611	59.672	2.121	25.702	1.00 24.60
1	MOTA	3169	CG	MET	611	59.215	2.462	24.303	1.00 24.10
1	ATOM	3170	SD	MET	611	59.972	4.035	23.821	1.00 26.77
3	MOTA	3171	CE	MET	611	59.546	5.0 90	25.184	1.00 19.21
1	MOTA	3172	C	MET	611	61.600	2.071	27.314	1.00 27.68
1	MOTA	3173	0	MET	611	61.891	3.128	27.865	1.00 28.22
7	MOTA	3174	N	GLU	612	61.562	0.908	27.967	1.00 31.07
7	MOTA	3175	CA	GLU	612	61.955	0.791	29.382	1.00 35.25
7	MOTA	3176	CB	GLU	612	61.809	-0.659	29.872	1.00 34.95
F	MOTA	3177	CG	GLU	612	62.383	-0.937	31.257	1.00 31.64
F	MOTA	3178	CD	GLU	612	62.392	-2.422	31.631	1.00 32.34
	MOTA	3179		GLU	612	62.599	-3.275	30.738	1.00 30.09
	MOTA	3180		GLU	612	62.226	-2.737	32.831	1.00 33.90
	MOTA	3181	C	GLU	612	63.409	1.252	29.468	1.00 37.14
	MOTA	3182	0	GLU	612	63.791	1.995	30.390	1.00 35.60
	MOTA	3183	N	TYR	613	64.196	0.868	28.457	1.00 37.89
	MOTA	3184	CA	TYR	613	65.601	1.247	28.392	1.00 36.68
	TOM	3185	CB	TYR	613	66.328	0.531	27.246	1.00 34.23
	TOM	3186	CG	TYR	613	67.801	0.888	27.175	1.00 36.59
	TOM	3187	CD1		613	68.734	0.263	28.005	1.00 36.83
	TOM	3188		TYR	613	70.090	0.649	28.013	1.00 34.51
	MOT	3189	CD2		613	68.252	1.909	26.339	1.00 35.28
	MOTA	3190	CE2		613	69.596	2.306	26.340	1.00 34.09
	TOM	3191	CZ	TYR	613	70.512	1.674	27.181	1.00 35.91
	MOTA MOTA	3192 3193	OH	TYR	613	71.826	2.089	27.212	1.00 29.78
	TOM	3194	О С	TYR TYR	613	65.724	2.760	28.233	1.00 37.58
	TOM	3195	N	LEU	613 614	66.362	3.414	29.056	1.00 39.84
	TOM	3196	CA	LEU	614	65.081 65.156	3.326	27.214	1.00 35.53
	TOM	3197	CB	LEU	614	64.314	4.766 5.157	26.988	1.00 34.58
	TOM	3198	CG	LEU	614	64.760	4.601	25.781 24.429	1.00 31.88
	TOM	3199	CD1		614	63.783	5.016	23.346	1.00 29.62 1.00 29.19
	TOM	3200	CD2		614	66.134.	5.133	24.111	1.00 23.13
	TOM	3201	C	LEU	614	64.698	5.538	28.218	1.00 36.38
	TOM	3202	0	LEU	614	65.325	6.525	28.618	1.00 33.81
A	TOM	3203	N	ALA	615	63.608	5.076	28.821	1.00 38.08
A	TOM	3204	CA	ALA	615	63.066	5.711	30.018	1.00 41.01
A	MOT	3205	CB	ALA	615	61.767	5.018	30.444	1.00 42.33
A	MOT	3206	С	ALA	615	64.099	5.683	31.147	1.00 40.47
A	MOT	3207	0	ALA	615	64.291	6.690	31.831	1.00 41.28
A	MOT	3208	N	SER	616	64.788	4.553	31.307	1.00 38.78
A	TOM	3209	CA	SER	616	65.806	4.441	32.347	1.00 40.97
A	TOM	3210	CB	SER	616	66.354	3.009	32.454	1.00 37.82
	TOM	3211	OG	SER	616	67.172	2.651	31.359	1.00 34.73
A	TOM	3212	С	SER	616	66.941	5.416	32.061	1.00 42.68
	TOM	3213	0	SER	616	67.714	5.769	32.957	1.00 45.78
A	TOM	3214	N	LYS	617	67.015	5.869	30.815	1.00 40.92
A	TOM	3215	CA	LYS	617	68.025	6.816	30.380	1.00 38.04
	TOM	3216	CB	LYS	617	68.541	6.411	29.003	1.00 38.25
A	MOT	3217	CG	LYS	617	69.293	5.111	29.021	1.00 36.40
A	TOM	3218	CD	LYS	617	70.421	5.221	29.992	1.00 38.14

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MOTA	3219	CE	LYS	617	71.215	3.941	30.086	1.00	38.43	
MOTA	3220	NZ	LYS	617	72.530	4.210	30.751	1.00	43.07	
ATOM	3221	C	LYS	617	67.475	8.242	30.350	1.00	38.42	
ATOM	3222	0	LYS	617	68.072	9.133	29.744	1.00	41.37	
ATOM	3223	N	LYS	618	66.323	8.444	30.985	1.00	37.25	
ATOM	3224	CA	LYS	618	65.674	9.743	31.067	1.00	36.75	
MOTA	3225	CB	LYS	618	66.653	10.780	31.632	1.00	43.27	
MOTA	3226	CG	LYS	618	67.340	10.392	32.938	1.00	51.59	
MOTA	3227	CD	LYS	618	66.377	10.361	34.092	1.00	61.24	
ATOM	3228	CE	LYS	618	67.070	9.945	35.373	1.00	67.83	
MOTA	3229	NZ	LYS	618	66.105	10.039	36.510		75.22	
ATOM	3230	С	LYS	618	65.167	10.222	29.706	1.00	36.61	
ATOM	3231	0	LYS	618	64.856	11.396	29.535		35.94	
ATOM	3232	N	CYS	619	65.058	9.308	28.751		36.26	
ATOM	3233	CA	CYS	619	64.603	9.666	27.412		33.41	
ATOM	3234	CB	CYS	619	65.351	8.843	26.365	1.00	32.17	
ATOM	3235	SG	CYS	619	65.006	9.223	24.650	1.00	26.92	
ATOM	3236	С	CYS	619	63.108	9.546	27.194	1.00	32.29	
ATOM	3237	0	CYS	619	62.510	8.472	27.373	1.00	29.13	
ATOM	3238	N	ILE	620	62.515	10.679	26.827	1.00	.31.60	
ATOM	3239	CA	ILE	620	61.091	10.763	26.528	1.00	31.21	
ATOM	3240	CB	ILE	620	60.435	11.966	27.212	1.00	29.57	
MOTA	3241	CG2	ILE	620	58.955	12.031	26.860	1.00	31.49	
MOTA	3242	CG1	ILE	620	60.578	11.848	28.727	1.00	27.85	
ATOM	3243	CD1	ILE	620	60.065	13.046	29.463	1.00	26.50	
MOTA	3244	С	ILE	620	61.034	10.972	25.018	1.00	32.18	
ATOM	3245	0	ILE	620	61.481	11.993	24.512	1.00	33.18	
MOTA	3246	N	HIS	621	60.472	9.990	24.318	1.00	31.93	
MOTA	3247	CA	HIS	621	60.354	9.970	22.864	1.00	32.59	
ATOM	3248	CB	HIS	621	59.933	8.552	22.420	1.00	29.51	
ATOM	3249	CG	HIS	621	60.076	8.288	20.951	1.00	27.45	
MOTA	3250	CD2	HIS	621	60.663	7.262	20.286	1.00	25.84	
MOTA	3251	ND1	HIS	621	59.528	9.106	19.979	1.00	25.20	
ATOM	3252	CE1	HIS	621	59.774	8.596	18.783	1.00	25.07	
MOTA	3253	NE2	HIS	621	60.456	7.473	18.942	1.00	23.24	
MOTA	3254	С	HIS	621	59.365	10.992	22.320	1.00	35.31	
ATOM	3255	0	HIS	621	59.555	11.481	21.220	1.00	39.24	
MOTA	3256	N	ARG	622	58.256	11.216	23.028	1.00	36.50	
ATOM	3257	CA	ARG	622	57.225	12.169	22.580	1.00	35.78	
ATOM	3258	CB	ARG	622	57.783	13.582	22.462	1.00	32.55	
ATOM	3259	CG	ARG	622	58.211	14.156	23.778	1.00	30.54	
ATOM	3260	CD	ARG	622	58.799	15.551	23.635	0.50	27.28	
ATOM	3261	NE	ARG	622	59.249	16.043	24.930	0.50	24.53	
MOTA	3262	CZ	ARG	622	60.409	15.707	25.499	0.50	27.85	
MOTA	3263	NH1	ARG	622	61.249	14.883	24.877	0.50	27.61	
MOTA	3264	NH2	ARG	622	60.711	16.158	26.714	0.50	25.34	
MOTA	3265	C	ARG	622	56.447	11.806	21.297	1.00	35.76	
ATOM	3266	0	ARG	622	55.438	12.430	20.999	1.00	36.61	
ATOM	3267	N	ASP	623	56.923	10.818	20.537	1.00	34.69	
MOTA	3268	CA	ASP	623	56.197	10.400	19.335	1.00	34.09	
ATOM	3269	CB	ASP	623	56.628	11.171	18.081	1.00	34.77	
ATOM	3270	CG	ASP	623	55.727	10.869	16.863		43.51	

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ATOM	3271	OD1	ASP	623	56.213	10.992	15.714	1.00 47.45
MOTA	3272		ASP	623	54.538	10.509	17.032	1.00 47.51
ATOM	3273	C	ASP	623	56.321	8.903	19.115	1.00 32.51
ATOM	3274	0	ASP	623	56.635	8.435	18.025	1.00 31.80
MOTA	3275	N	LEU	624	56.081	8.135	20.164	1.00 31.80
MOTA	3276	CA	LEU	624	56.152	6.689	20.030	1.00 31.07
MOTA	3277	CB	LEU	624	56.133	6.029	21.403	1.00 28.11
ATOM	3278	CG	LEU	624	55.98 3	4.510	21.460	1.00 27.88
ATOM	3279	CD1	LEU	624	57.108	3.809	20.700	1.00 23.96
ATOM	3280	CD2	LEU	624	56.001	4.088	22.912	1.00 29.50
ATOM	3281	С	LEU	624	54.954	6.238	19.187	1.00 32.04
MOTA	3282	0	LEU	624	53.805	6.564	19.505	1.00 36.02
ATOM	3283	N ·	ALA	625	55.224	5.561	18.076	1.00 28.91
ATOM	3284	CA	ALA	625	54.170	5.066	17.192	1.00 25.66
ATOM	3285	CB	ALA	625	53.707	6.170	16.289	1.00 23.37
ATOM	3286	С	ALA	625	54.800	3.948	16.389	1.00 27.71
MOTA	3287	0	ALA	625	56.022	3.841	16.355	1.00 29.77
ATOM	3288	N	ALA	626	53.982	3.107	15.758	1.00 29.46
MOTA	3289	CA	ALA	626	54.499	1.993	14.956	1.00 28.16
ATOM	3290	CB	ALA	626	53.350	1.155	14.401	1.00 28.02
ATOM	3291	С	ALA	626	55.366	2.504	13.831	1.00 26.78
ATOM	3292	0	ALA	626	56.329	1.859	13.454	1.00 26.69
ATOM	3293	N	ARG	627	55.022	3.680	13.314	1.00 26.09
ATOM	3294	CA	ARG	627	55. <i>777</i>	4.301	12.246	1.00 26.78
ATOM	3295	CB	ARG	627	55.134	5.637	11.837	1.00 27.01
ATOM	3296	CG	ARG	627	55.046	6.672	12.961	1.00 29.34
ATOM	3297	CD	ARG	627	54.552	8.037	12.477	1.00 34.26
ATOM	3298	NE	ARG	627	54.108	8.878	13.590	1.00 36.96
ATOM	3299	CZ	ARG	627	52.867	8.889	14.059	1.00 40.84
ATOM	3300	NH1		627	51.942	8.114	13.515	1.00 42.56
ATOM	.3301	NH2		627	52.552	9.634	15.108	1.00 45.20
ATOM	3302	C	ARG	627	57.209	4.549	12.711	1.00 29.11
ATOM	3303	0	ARG	627	58.137	4.468	11.911	1.00 30.39
ATOM	3304	N	ASN	628	57.385	4.804	14.010	1.00 30.37
ATOM	3305	CA	ASN	628	58.689	5.092	14.596	1.00 27.02
MOTA	3306	CB	ASN	628	58.578	6.226	15.611	1.00 24.35
ATOM	3307	CG	ASN	628	58.383	7.571	14.941	1.00 25.95
MOTA	3308	OD1		628	58.992	7.865	13.924	1.00 32.01
MOTA MOTA	3309	ND2		628	57.522	8.391	15.503	1.00 24.34
ATOM	3310	C	ASN	628	59.437	3.903	15.185	1.00 26.74
	3311	0	ASN	628	60.378	4.062	15.972	1.00 28.49
ATOM	3312	N	VAL	629	58.998	2.712	14.802	1.00 27.34
ATOM	3313	CA	VAL	629	59.621	1.450	15.224	1.00 24.94
ATOM ATOM	3314	CB	VAL	629	58.589	0.522	15.906	1.00 22.20
	3315	CG1		629	59.169	-0.883	16.089	1.00 18.03
ATOM	3316	CG2		629	58.158	1.121	17.244	1.00 18.34
ATOM	3317	С	VAL	629	60.077	0.805	13.918	1.00 26.84
ATOM	3318	0	VAL	629	59.284	0.679	12.978	1.00 26.50
ATOM	3319	N Ch	LEU	630	61.352	0.469	13.809	1.00 27.66
ATOM	3320	CA	LEU	630	61.862	-0.158	12.601	1.00 30.14
ATOM	3321	CB	LEU	630	63.105	0.577	12.122	1.00 28.00
ATOM	3322	CG	LEU	630	62.856	2.086	12.027	1.00 26.06

ATOM 630 3323 CD1 LEU 64.150 2.831 11.832 1.00 23.44 MOTA 3324 CD2 LEU 630 10.901 61.880 2.381 1.00 27.72 ATOM 3325 С LEU 630 62.145 -1.627 12.889 1.00 32.90 3326 MOTA 0 LEU 630 62.437 -1.982 14.029 1.00 33.06 3327 VAL MOTA N 631 61.991 -2.478 11.873 1.00 34.83 **ATOM** 3328 CA VAL 631 62.195 -3.928 12.006 1.00 33.02 MOTA 3329 CB VAL 631 60.915 -4.700 11.584 1.00 30.92 **ATOM** 3330 CG1 VAL 631 61.071 -6.208 11.842 1.00 27.66 MOTA 3331 CG2 VAL 631 59.724 -4.161 12,332 1.00 24.46 **ATOM** 3332 С VAL 631 63.371 -4.415 11.161 1.00 35.77 MOTA 3333 0 VAL 631 63.428 1.00 37.57 -4.171 9.954 MOTA 3334 N THR 632 64.319 -5.098 11.797 1.00 37.96 MOTA 3335 CA THR 632 65.511 -5.599 11.096 1.00 39.06 **ATOM** 3336 CB THR 632 66.675 -5.820 12.066 1.00 35.55 ATOM 3337 OG1 THR 632 66.368 -6.903 12.955 1.00 35.76 ATOM 3338 CG2 THR 632 66.928 -4.561 12.867 1.00 35.06 **ATOM** 3339 С THR 632 65.283 -6.893 10.331 1.00 40.66 **ATOM** 3340 0 THR 632 64.238 -7.515 10.466 1.00 41.79 **ATOM** 3341 N GLU 633 66.282 -7.307 9.556 1.00 43.40 MOTA 3342 CA GLU 633 66.219 -8.540 8.768 1.00 45.33 MOTA 3343 CB GLU 633 67.501 -8.689 7.942 1.00 48.67 MOTA 3344 CG GLU 633 67.496 -9.791 6.864 1.00 54.70 MOTA 3345 CD GLU 633 66.599 -9.506 5.647 1.00 58.16 MOTA 3346 OE1 GLU 633 65.933 -8.452 5.567 1.00 60.68 **ATOM** 3347 OE2 GLU 633 66.566 -10.369 4.747 1.00 60.14 **ATOM** 3348 С GLU 633 66.011 -9.774 9.648 1.00 46.02 MOTA 3349 0 GLU 633 65.637 -10.834 9.156 1.00 46.75 MOTA 3350 N ASP 634 66.278 -9.648 10.944 1.00 46.45 MOTA 3351 CA ASP 634 65.085 -10.774 11.843 1.00 46.14 **ATOM** 3352 ASP CB 634 67.316 -10.995 12.724 1.00 52.89 **ATOM** 3353 CG ASP 634 68.570 -11.399 11.929 1.00 59.65 **ATOM** 3354 OD1 ASP 11.328 1.00 59.91 634 68.593 -12.499 MOTA 3355 OD2 ASP 634 69.546 -10.608 11.918 1.00 62.29 MOTA 3356 С **ASP** 634 64.850 -10.549 12.708 1.00 45.75 MOTA 3357 0 ASP 634 64.729 -11.138 13.776 1.00 46.38 MOTA 3358 N ASN 635 63.940 -9.697 12.235 1.00 45.92 **ATOM** 3359 CA ASN 635 62.690 -9.367 12.915 1.00 44.36 61.750 -10.583 **ATOM** 3360 CB ASN 635 12.972 1.00 46.62 3361 **ATOM** CG ASN 635 61.409 -11.116 11.597 1.00 47.56 **ATOM** 3362 OD1 ASN 635 60.750 -10.453 10.800 1.00 50.54 MOTA 3363 ND2 ASN 635 61.876 -12.314 11.305 1.00 47.75 **ATOM** 3364 С ASN 635 62.833 -8.763 14.308 1.00 42.78 MOTA 3365 0 ASN 635 62.028 -9.045 15.189 1.00 44.56 MOTA 3366 N VAL 636 63.849 -7.927 14.503 1.00 41.03 MOTA 3367 CA VAL 636 64.071 -7.291 15.797 1.00 36.87 MOTA 3368 CB VAL 636 65.584 -7.162 16.083 1.00 35.99 **ATOM** 3369 CG1 VAL 636 65.839 -6.347 17.354 1.00 34.01 ATOM 3370 CG2 VAL 636 66.184 -8.535 16.226 1.00 33.65 MOTA 3371 C VAL 636 63.434 -5.908 15.782 1.00 34.79 -5.131 MOTA 3372 0 VAL 636 63.657 14.854 1.00 36.58 ATOM 3373 N MET 637 62.600 -5.625 16.773 1.00 32.04 **MOTA** 3374 CA MET 637 61.940 -4.331 16.887 1.00 31.14

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ATOM	3375	CB	MET	637	60.734	-4.427	17.817	1.00 35.49
MOTA	3376	CG	MET	637	59.702	-5.501	17.437	1.00 37.77
MOTA	3377	SD	MET	637	58.835	-5.257	15.857	1.00 39.62
ATOM	3378	CE	MET	637	59.122	-6.864	15.035	1.00 34.87
ATOM	3379	С	MET	637	62.935	-3.342	17.479	1.00 29.95
ATOM	3380	0	MET	637	63.525	-3.612	18.526	1.00 26.48
MOTA	3381	N	LYS	638	63.044	-2.167	16.861	1.00 29.03
ATOM	3382	CA	LYS	638	63.977	-1.133	17.293	1.00 24.64
MOTA	3383	CB	LYS	638	65.214	-1.150	16.390	1.00 22.85
MOTA	3384	CG	LYS	638	66.145	-2.305	16.655	1.00 17.56
ATOM	3385	CD	LYS	638	67.307	-2.274	15.707	1.00 19.48
ATOM	3386	CE	LYS	638	68.369	-3.242	16.146	1.00 17.71
ATOM	3387	NZ	LYS	638	68.931	-2.895	17.473	1.00 24.81
MOTA	3388	С	LYS	638	63.367	0.260	17.270	1.00 24.75
ATOM	3389	0	LYS	638	62.987	0.740	16.203	1.00 24.35
MOTA	3390	N	ILE	639	63.277	0.905	18.437	1.00 24.63
ATOM	3391	CA	ILE	639	62.734	2.256	18.536	1.00 24.75
ATOM	3392	CB	ILE	639	62.699	2.789	19.993	1.00 23.98
ATOM	3393	CG2	ILE	639	61.916	4.094	20.046	1.00 21.11
MOTA	3394	CG1	ILE	639	62.127	1.740	20.963	1.00 26.06
ATOM	3395	CD1	ILE	639	60.680	1.392	20.758	1.00 28.45
ATOM	3396	C	ILE	639	63.656	3.198	17.774	1.00 26.36
MOTA	3397	0	ILE	639	64.884	3.161	17.947	1.00 25.06
ATOM	3398	N	ALA	640	63.07 3	4.072	16.963	1.00 26,70
ATOM	3399	CA	ALA	640	63.857	5.037	16.202	1.00 27.85
ATOM	3400	CB	ALA	640	63.683	4.777	14.736	1.00 27.66
ATOM	3401	C	ALA	640	63.380	6.449	16.548	1.00 29.56
MOTA	3402	0	ALA	640	62.307	6.608	17.136	1.00 29.82
MOTA	3403	N	ASP	641	64.174	7.456	16.180	1.00 28.74
ATOM	3404	CA	ASP	641	63.863	8.874	16.415	1.00 32.13
ATOM	3405	CB	ASP	641	62.662	9.310	15.574	1.00 35.25
ATOM	3406	CG	ASP	641	63.024	9.555	14.121	1.00 38.54
ATOM	3407		ASP	641	64.149	9.170	13.716	1.00 39.85
ATOM	3408		ASP	641	62.192	10.144	13.394	1.00 41.38
ATOM	3409	C	ASP	641	63.661	9.311	17.862	1.00 30.61
ATOM	3410	0	ASP	641	63.012	10.323	18.140	1.00 29.45
ATOM	3411	N	PHE	642	64.265	8.567	18.776	1.00 30.96
MOTA MOTA	3412	CA	PHE	642	64.155	8.860	20.195	1.00 31.21
ATOM	3413	CB	PHE	642	64.447	7.597	21.013	1.00 27.06
	3414	CG	PHE	642	65.806	7.008	20.749	1.00 24.27
ATOM ATOM	3415 3416		PHE	642 642	66.930	7.476	21.419	1.00 22.36
ATOM	3417	CE1			65.962	5.978	19.838	1.00 24.87
ATOM	3418			642	68.179	6.928	21.190	1.00 23.19
ATOM		CE2		642	67.205	5.420	19.603	1.00 23.65
ATOM	3419 3420	CZ ·	PHE PHE	642	68.323	5.898	20.282	1.00 22.95
				642	65.069	10.007	20.623	1.00 34.88
ATOM ATOM	3421	0 N	PHE	642	64.920	10.549	21.729	1.00 34.84
ATOM	3422	N	GLY	643	66.000	10.377	19.737	1.00 36.20
	3423	CA	GLY	643	66.934	11.450	20.032	1.00 35.47
ATOM	3424	C	GLY	643	66.728	12.720	19.232	1.00 37.62
ATOM	3425	0	GLY	643	67.581	13.593	19.269	1.00 39.16
MOTA	3426	N	LEU	644	65.609	12.837	18.517	1.00 39.68

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ATOM	3427	CA	LEU	644	65.328	14.029	17.712	1.00 43.09
MOTA	3428	CB	LEU	644	64.074	13.843	16.860	1.00 40.78
MOTA	3429	CG	LEU	644	64.076	12.876	15.681	1.00 36.94
MOTA	3430	CD1	LEU	644	62.790	13.076	14.901	1.00 37.34
MOTA	3431	CD2	LEU	644	65.240	13.157	14.783	1.00 37.72
ATOM	3432	С	LEU	644	65.154	15.261	18.591	1.00 47.32
ATOM	3433	0	LEU	644	64.639	15.170	19.702	1.00 50.33
ATOM	3434	N	ALA	645	65.598	16.406	18.088	1.00 51.23
ATOM	3435	CA	ALA	645	65.507	17.662	18.820	1.00 52.97
ATOM	3436	CB	ALA	645	66.367	18.703	18.151	1.00 54.12
ATOM	3437	С	ALA	645	64.060	18.137	18.910	1.00 53.00
MOTA	3438	0	ALA	645	63.591	18.528	19.977	1.00 53.59
MOTA	3439 -	·N	ASP	652	52.356	21.675	14.855	1.00 79.51
MOTA	3440	CA	ASP	652	51.194	21.821	13.993	1.00 78.74
MOTA	3441	CB	ASP	652	51.625	22.021	12.531	1.00 78.30
MOTA	3442	CG	ASP	6 52	50.459	22.358	11.608	1.00 77.64
ATOM	3443	OD1	ASP	652	49.473	22.968	12.079	1.00 77.67
MOTA	3444	OD2	ASP	652	50.526	22.029	10.410	1.00 78.25
ATOM	3445	С	ASP	652	50.339	20.569	14.125	1.00 78.92
ATOM	3446	0	ASP	652	50.645	19.529	13.539	1.00 79.36
MOTA	3447	N	TYR	653	49.262	20.682	14.892	1.00 79.17
MOTA	3448	CA	TYR	653	48.357	19.560	15.111	1.00 80.23
ATOM	3449	СВ	TYR	653	47.283	19.932	16.136	1.00 81.36
MOTA	3450	CG	TYR	653	47.790	20.060	17.557	1.00 84.51
ATOM	3451	CD1	TYR	653	46.998	20.649	18.544	1.00 86.09
ATOM	3452	CE1	TYR	653	47.443	20.751	19.865	1.00 88.05
ATOM	3453	CD2	TYR	653	49.049	19.576	17.925	1.00 86.22
ATOM	3454	CE2	TYR	653	49.504	19.673	19.242	1.00 87.14
ATOM	3455	CZ	TYR	653	48.698	20.260	20.207	1.00 88.37
MOTA	3456	ОН	TYR	653	49.146	20.351	21.510	1.00 88.82
ATOM	3457	С	TYR	653	47.687	19.098	13.827	1.00 80.07
ATOM	3458	0	TYR	653	47.170	17.983	13.752	1.00 81.23
ATOM	3459	N	TYR	654	47.716	19.953	12.813	1.00 79.01
ATOM	3460	CA	TYR	654	47.082	19.640	11.544	1.00 78.81
ATOM	3461	CB	TYR	654	46.378	20.884	11.008	1.00 78.48
ATOM	3462	CG	TYR	654	45.358	21.422	11.982	1.00 78.53
MOTA	3463	CD1	TYR	654	45.752	21.948	13.213	1.00 77.46
MOTA	3464	CE1	TYR	654	44.822	22.382	14.146	1.00 78.94
MOTA	3465	CD2	TYR	654	43.997	21.350	11.704	1.00 80.18
ATOM	3466	CE2	TYR	654	43.054	21.785	12.632	1.00 82.55
MOTA	3467	CZ	TYR	654	43.473	22.295	13.851	1.00 80.98
MOTA	3468	OH	TYR	654	42.548	22.703	14.785	1.00 82.29
MOTA	3469	С	TYR	654	48.010	19.042	10.499	1.00 79.04
ATOM	3470	0	TYR	654	47.575	18.720	9.393	1.00 80.09
MOTA	3471	N	LYS	655	49.277	18.859	10.848	1.00 78.74
MOTA	3472	CA	LYS	655	50.217	18.282	9.906	1.00 80.69
MOTA	3473	СВ	LYS	655	51.651	18.687	10.247	1.00 83.97
ATOM	3474	CG	LYS	655	52.674	18.124	9.281	1.00 89.76
MOTA	3475	CD	LYS	655	54.084	18.565	9.611	1.00 93.90
ATOM	3476	CE	LYS	655	55.075	17.844	8.708	1.00 97.62
MOTA	3477	NZ	LYS	655	56.489	18.177	9.038	1.00101.35
MOTA	3478	С	LYS	655	50.070	16.763	9.922	1.00 80.98

ATOM	3479	0	LYS	655	50.187	16.130	10.975	1.00 80.95
ATOM	3480	N	LYS	656	49.766	16.194	8.759	1.00 81.29
MOTA	3481	CA	LYS	656	49.599	14.749	8.630	1.00 81.06
MOTA	3482	CB	LYS	656	48.723	14.426	7.423	1.00 81.40
ATOM	3483	CG	LYS	656	47.258	14.779	7.596	1.00 81.60
ATOM	3484	CD	LYS	656	46.518	14.565	6.295	1.00 84.93
ATOM	3485	CE	LYS	656	45.019	14.620	6.493	1.00 87.78
ATOM	3486	NZ	LYS	656	44.291	14.565	5.183	1.00 91.78
MOTA	3487	С	LYS	656	50.940	14.026	8.513	1.00 80.44
ATOM	3488	0	LYS	6 56	51.923	14.596	8.032	1.00 80.35
ATOM	3489	N	GLY	660	49.197	9.779	5.831	1.00 57.41
ATOM	3490	CA	GLY	660	48.231	10.860	5.961	1.00 55.59
ATOM	3491	C	GLY	660	47.492	10.866	7.285	1.00 53.27
ATOM	3492	0	GLY	660	46.403	11.432	7.388	1.00 53.03
MOTA	3493	N	ARG	661	48.080	10.222	8.288	1.00 51.92
MOTA	3494	CA	ARG	661	47.477	10.155	9.617	1.00 48.40
ATOM	3495	CB	ARG	661	47.900	8.861	10.338	1.00 50.20
ATOM	3496	CG	ARG	661	47.612	7.566	9.563	1.00 49.76
ATOM	3497	CD	ARG	661	47.801	6.331	10.456	1.00 52.48
ATOM	3498	NE	ARG	661	47.691	5.061	9.734	1.00 52.60
MOTA	3499	CZ	ARG	661	47.955	3.866	10.264	1.00 50.93
ATOM	3500	NH1	ARG	661	48.343	3.760	11.529	1.00 48.54
ATOM	3501	NH2	ARG	661	47.836	2.772	9.523	1.00 52.75
ATOM	3502	C	ARG	661	47.894	11.379	10.439	1.00 43.91
ATOM	3503	0	ARG	661	48.833	12.096	10.063	1.00 43.23
ATOM	3504	N	LEU	662	47.194	11.618	11.537	1.00 40.56
ATOM	3505	CA	LEU	662 .	47.496	12.735	12.428	1.00 37.52
ATOM	3506	СВ	LEU	662	46.220	13.496	12.789	1.00 33.26
ATOM	3507	CG	LEU	662	45.485	14.281	11.696	1.00 31.29
ATOM	3508	CD1	LEU	662	44.084	14.621	12.158	1.00 24.03
ATOM	3509	CD2	LEU	662	46.261	15.535	11.358	1.00 28.65
ATOM	3510	С	LEU	662	48.154	12.237	13.712	1.00 36.78
ATOM	3511	0	LEU	662	47.515	11.570	14.536	1.00 37.27
ATOM	3512	N	PRO	663	49.448	12.549	13.895	1.00 36.46
ATOM	3513	CD	PRO	663	50.320	13.216	12.914	1.00 38.35
ATOM	3514	CA	PRO	663	50.224	12.148	15.070	1.00 35.98
ATOM	3515	СВ	PRO	663	51.537	12.887	14.872	1.00 34.95
ATOM	3516	CG	PRO	663	51.702	12.836	13.403	1.00 39.18
MOTA	3517	С	PRO	663	49.569	12.499	16.398	1.00 35.53
ATOM	3518	0	PRO	663	49.779	11.814	17.399	1.00 38.34
ATOM	3519	N	VAL	664	48.759	13.558	16.414	1.00 30.34
ATOM	3520	CA	VAL	664	48.080	13.964	17.632	1.00 30.18
ATOM	3521	СВ	VAL	664	47.195	15.242	17.427	1.00 30.10
ATOM	3522	CG1		664	48.060	16.409	17.038	1.00 28.93
ATOM	3523	CG2		664	46.143	15.038	16.345	
ATOM	3524	C	VAL	664	47.268	12.787	18.172	1.00 34.42
ATOM	3525	0	VAL	664	47.288	12.787		1.00 29.48
ATOM	3526	N	LYS	665			19.388	1.00 30.41
ATOM	3527	CA	LYS	665	46.873	11.883	17.282	1.00 29.29
ATOM	352 <i>1</i> 3528	CB			46.105	10.704	17.668	1.00 28.55
ATOM			LYS	665	45.517	10.037	16.423	1.00 26.97
	3529	CG	LYS	665	44.415	10.873	15.786	1.00 27.88
ATOM	3530	CD	LYS	665	43.979	10.366	14.418	1.00 29.41

ATOM	3531	CE	LYS	665	42.785	11.162	13.899	1.00 26.35	
MOTA	3532	NZ	LYS	665	42.363	10.809	12.508	1.00 26.16	
ATOM	3533	С	LYS	665	46.890	9.730	18.556	1.00 28.81	
MOTA	3534	0	LYS	665	46.315	8.802	19.113	1.00 29.38	
MOTA	3535	N	TRP	666	48.181	9.976	18.736	1.00 28.98	
ATOM	3536	CA	TRP	666	49.005	9.128	19.599	1.00 31.67	
ATOM	3537	CB	TRP	666	50.323	8.755	18.913	1.00 29.46	
ATOM	3538	CG	TRP	666	50.205	7.582	17.977	1.00 28.92	
ATOM	3539	CD2	TRP	666	49.676	7.603	16.642	1.00 27.62	
ATOM	3540	CE2	TRP	666	49.740	6.276	16.162	1.00 27.15	
MOTA	3541	CE3	TRP	666	49.151	8.607	15.818	1.00 25.27	
MOTA	3542	CD1	TRP	666	50.565	6.289	18.238	1.00 24.30	
MOTA	3543	NE1	TRP	·· 666··	50.287	5.506	17.147	1.00 27.82	
ATOM	3544	CZ2	TRP	666	49.295	5.930	14.872	1.00 26.95	
ATOM	3545	CZ3	TRP	666	48.707	8.256	14.536	1.00 25.95	
MOTA	3546	CH2	TRP	666	48.778	6.929	14.081	1.00 28.35	
MOTA	3547	С	TRP	666	49.316	9.836	20.907	1.00 33.46	
ATOM	3548	0	TRP	666	49.790	9.219	21.867	1.00 34.77	
ATOM	3549	N	MET	667	49.021	11.128	20.947	1.00 35.61	
ATOM	3550	CA	MET	667	49.306	11.948	22.110	1.00 37.94	
ATOM	3551	CB	MET	667	49.308	13.419	21.723	1.00 40.22	
ATOM	3552	CG	MET	667	50.606	13.939	21.150	1.00 40.77	
MOTA	3553	SD	MET	667	50.479	15.723	20.906	1.00 44.04	
MOTA	3554	CE	MET	667	50.932	15.858	19.204	1.00 39.07	
MOTA	3555	C	MET	667	48.432	11.775	23.346	1.00 39.61	
ATOM	3556	0	MET	667	47.211	11.672	23.255	1.00 42.46	
MOTA	3557	N	ALA	668	49.072	11.820	24.505	1.00 38.46	
ATOM	3558	CA	ALA	66B	48.383	11.704	25.773	1.00 37.78	
ATOM	3559	CB	ALA	668	49.388	11.473	26.894	1.00 38.21	
MOTA	3560	C	ALA	668	47.666	13.033	25.966	1.00 37.46	
MOTA	3561	0	ALA	668	48.156	14.072	25.521	1.00 35.74	
MOTA	3562	N	PRO	669	46.521	13.027	26.665	1.00 37.55	
MOTA	3563	CD	PRO	669	45.868	11.840	27.243	1.00 38.19	
MOTA	3564	CA	PRO	669	45.723	14.229	26.923	1.00 39.30	
MOTA	3565	СВ	PRO	669	44.638	13.708	27.864	1.00 39.82	
ATOM	3566	CG	PRO	669	44.444	12.301	27.379	1.00 39.13	
MOTA	3567	С	PRO	669	46.517	15.391	27.535	1.00 40.55	
ATOM	3568	0	PRO	669	46.442	16.523	27.056	1.00 39.87	
MOTA	3569	N	GLU	670	47.303	15.113	28.569	1.00 41.15	
ATOM	3570	CA	GLU	670	48.096	16.169	29.200	1.00 42.80	
MOTA	3571	CB	GLU	670	48.776	15.657	30.464	1.00 42.97	
MOTA	3572	CG	GLU	670	49.928	14.705	30.205	1.00 42.82	
ATOM	3573	CD	GLU	670	49.506	13.252	30.150	1.00 44.16	
ATOM	3574	OE1	GLU	670	50.395	12.384	30.257	1.00 40.43	
ATOM	3575	OE2	GLU	670	48.297	12.974	30.013	1.00 46.36	
MOTA	3576	С	GLU	670	49.145	16.795	28.276	1.00 43.00	
ATOM	3577	0	GLU	670	49.435	17.979	28.380	1.00 40.37	
ATOM	3578	N	ALA	671	49.697	15.999	27.367	1.00 44.03	
ATOM	3579	CA	ALA	671	50.708	16.495	26.440	1.00 44.90	
ATOM	3580	СВ	ALA	671	51.460	15.333	25.814	1.00 42.47	
ATOM	3581		ALA	671	50.063	17.364	25.361	1.00 47.79	
ATOM	3582	0	ALA	671	50.602	18.398	24.977	1.00 47.27	
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MOTA	3583	N	LEU	672	48.877	16.952	24.922	1.00	51.20
ATOM	3584	CA	LEU	672	48.131	17.650	23.881	1.00	52.90
ATOM	3585	CB	LEU	672	47.092	16.685	23.288	1.00	54.84
MOTA	3586	CG	LEU	672	46.307	17.010	22.015	1.00	57.19
ATOM	3587	CD1	LEU	672	47.230	17.328	20.869	1.00	57.53
MOTA	3588	CD2	LEU	672	45.443	15.813	21.659	1.00	56.95
MOTA	3589	C	LEU	672	47.456	18.913	24.445	1.00	53.45
MOTA	3590	0	LEU	672	47.502	19.988	23.841	1.00	52.71
MOTA	3591	N	PHE	673	46.866	18.777	25.627	1.00	53.82
MOTA	3592	CA	PHE	673	46.179	19.878	26.281	1.00	55.95
ATOM	3593	CB	PHE	673	44.974	19.340	27.060	1.00	53.37
ATOM	3594	CG	PHE	673	43.967	18.612	26.200	1.00	52.79
ATOM	3595		PHE	673	43.477	17.368	26.580	1:00	54.64
ATOM	3596		PHE	673	43.491	19.173	25.022	1.00	53.89
ATOM	3597		PHE	673	42.530	16.702	25.808	1.00	55.44
ATOM	3598	CE2	PHE	673	42.540	18.507	24.239	1.00	54.80
ATOM	3599	CZ	PHE	673	42.062	17.269	24.637	1.00	54.86
ATOM	3600	C	PHE	673	47.071	20.733	27.200	1.00	58.97
ATOM	3601	0	PHE	673	47.084	21.959	27.095	1.00	60.79
ATOM	3602	N	ASP	674	47.832	20.086	28.077	1.00	60.63
ATOM	3603	CA	ASP	674	48.698	20.798	29.026	1.00	61.52
ATOM	3604	CB	ASP	674	48.638	20.137	30.410	1.00	61.39
MOTA	3605	CG	ASP	674	47.247	20.143	31.010		62.87
ATOM	3606	OD1		674	46.706	19.039	31.246		62.99
ATOM	3607	OD2		674	46.698	21.239	31.253		63.55
ATOM	3608	C	ASP	674	50.176	20.998	28.618		61.58
ATOM ATOM	3609	O N	ASP	674	51.014	21.284	29.446		60.41
ATOM	3610	N	ARG	675	50.499	20.519	27.380		61.38
ATOM	3611 3612	CA	ARG	675	51.885	20.526	26.883	1.00	
ATOM	3613	CB CG	ARG	675	52.336	21.944	26.515		59.05
ATOM	3614	CD	ARG ARG	675 675	51.548	22.564	25.367		64.48
ATOM	3615	NE	ARG	675	52.036	23.967	25.014		68.61
ATOM	3616	CZ	ARG	675	53.348	23.969	24.359		69.16
ATOM	3617	NH1		675	54.076 53.622	25.061	24.145		68.19
ATOM	3618	NH2		675	55.265	26.250	24.531		66.97
ATOM	3619	C	ARG	675	52.849	24.965 19.885	23.564		67.00
ATOM	3620	0	ARG	675	54.002	20.300	27.892		57.27
ATOM	3621	N	ILE	676	52.356	18.867	28.033		57.05
ATOM	3622	CA	ILE	676	53.136	18.140	28.591 29.589		55.44 53.31
ATOM	3623	СВ	ILE	676	52.314	17.899	30.874		50.96
ATOM	3624	CG2		676	52.934	16.787	31.718		47.57
ATOM	3625	CG1		676	52.213	19.196	31.669		50.88
ATOM	3626	CD1		676	51.443	19.073	32.964		53.09
ATOM	3627	C	ILE	676	53.608	16.801	29.029		54.75
ATOM	3628	ō ·	ILE	676	52.810	15.891	28.824		57.06
ATOM	3629	N	TYR	677	54.902	16.681	28.777		53.61
ATOM	3630	CA	TYR	677	55.459	15.447	28.243		52.80
ATOM	3631	CB	TYR	677	56.332	15.747	27.023		53.40
ATOM	3632	CG	TYR	677	55.554	16.184	25.794		57.32
ATOM	3633	CD1		677	55.256	17.535	25.575		55.94
ATOM	3634	CEl		677	54.574	17.946	24.436		54.18
							~4.43U	1.00	~4.TO

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MOTA 3635 CD2 TYR 677 24.829 1.00 56.63 55.140 15.251 MOTA 3636 CE2 TYR 677 54.459 15.654 23.680 1.00 54.84 MOTA 3637 CZTYR 677 54.183 17.004 23.490 1.00 56.38 ATOM 3638 OH TYR 677 53.555 17.426 22.340 1.00 57.46 MOTA 3639 C TYR 677 56.268 14.713 29.304 1.00 51.49 **ATOM** 3640 0 TYR 677 57.186 15.283 29.904 1.00 52.65 **ATOM** 3641 N THR 678 55.881 13.471 29.579 1.00 48.54 **ATOM** 3642 CA THR 678 56.571 12.648 30.568 1.00 46.14 ATOM 3643 CB THR 678 55.776 12.597 31.910 1.00 47.34 MOTA 3644 OG1 THR 678 54.615 11.764 31.764 1.00 50.96 ATOM 3645 CG2 THR 678 55.346 13.996 1.00 47.47 32.345 MOTA 3646 С THR 678 56.742 11.218 30.041 1.00 43.21 MOTA 3647 0 THR 678 56.371 10.917 28.912 1.00 41.64 MOTA 3648 N HIS 679 57.334 10.351 30.854 1.00 42.21 MOTA 3649 HIS CA 679 57.507 8.969 30.456 1.00 39.96 ATOM 3650 CB HIS 679 58.410 8.216 31.428 1.00 39.23 MOTA 3651 CG HIS 679 59.833 8.677 31.418 1.00 43.24 ATOM 3652 CD2 HIS 679 60.501 9.505 32.253 1.00 43.12 **ATOM** 3653 ND1 HIS 1.00 42.63 679 60.759 8.236 30.498 MOTA 3654 CE1 HIS 679 61.938 8.762 30.774 1.00 42.66 MOTA 3655 NE2 HIS 679 61.807 9.539 31.832 1.00 43.80 ATOM 3656 С HIS 679 56.145 8.301 30.429 1.00 40.78 **ATOM** 3657 0 HIS 679 55.930 7.358 29.678 1.00 42.66 ATOM 3658 N GLN 680 55.227 8.803 31.254 1.00 40.26 **MOTA** 3659 CA GLN 680 53.881 8.261 31.324 1.00 39.10 ATOM 3660 CB GLN 680 53_187 B.664 32.625 1.00 39.23 ATOM 3661 CG GLN 680 53.762 7.980 33.874 1.00 41.07 ATOM 3662 CDGLN 680 53.813 6.450 33.770 1.00 39.96 **ATOM** 3663 OE1 GLN 680 52.818 5.762 33.993 1.00 39.53 **ATOM** 3664 NE2 GLN 680 54.990 5.919 33.464 1.00 32.85 MOTA 3665 С GLN 680 53.070 8.676 30.103 1.00 39.20 ATOM 3666 O GLN 680 52.194 7.933 29.656 1.00 39.29 MOTA 3667 N SER 681 53.368 9.843 29.531 1.00 38.01 MOTA 3668 CA SER 681 52.656 10.264 28.325 1.00 39.27 MOTA 3669 CB SER 681 52.979 11.712 27.968 1.00 40.93 MOTA 3670 OG SER 681 54.366 11.936 27.943 1.00 39.70 **ATOM** 3671 С SER 681 53.090 9.309 27.208 1.00 39.93 ATOM 3672 0 SER 681 52.285 8.953 26.335 1.00 40.46 ATOM 3673 N ASP 682 54.356 8.881 27.269 1.00 37.28 ATOM 3674 CA ASP 682 54.920 7.921 26.315 1.00 35.38 **MOTA** 3675 CB ASP 682 56.411 7.673 26.586 1.00 33.58 ATOM 3676 CG ASP 682 57.332 8.520 25.717 1.00 33.16 **ATOM** 3677 OD1 ASP 682 58.545 8.283 25.828 1.00 31.76 ATOM 3678 OD2 ASP 682 24.936 1.00 30.06 56.886 9.391 MOTA 3679 С ASP 682 54.178 6.599 26.463 1.00 34.70 MOTA 3680 0. ASP 682 54.012 5.868 25.488 1.00 35.67 MOTA 3681 N VAL 683 53.758 6.296 27.691 1.00 34.44 **MOTA** 3682 CA VAL 683 53.011 5.072 27.987 1.00 35.14 **ATOM** 3683 CB VAL 683 52.895 4.852 29.544 1.00 35.48 MOTA 3684 CG1 VAL 683 51.752 3.900 29.890 1.00 34.95 MOTA 3685 CG2 VAL 683 54.202 4.282 30.080 1.00 28.77 ATOM 3686 C VAL 683 51.638 5.091 27.279 1.00 32.81

	ATOM	3687	0	VAL	683	51.173	4.050	26.801	1.00 31.24
	ATOM	3688	N	TRP	684	51.018	6.271	27.187	1.00 30.88
	ATOM	3689	CA	TRP	684	49.731	6.426	26.502	1.00 31.79
	MOTA	3690	CB	TRP	684	49.189	7.849	26.679	1.00 34.88
	MOTA	3691	CG	TRP	684	47.972	8.173	25.833	1.00 37.61
	ATOM	3692	CD2	TRP	684	46.635	8.396	26.305	1.00 39.13
	ATOM	3693	CE2	TRP	684	45.851	8.741	25.184	1.00 38.42
	MOTA	3694	CE3	TRP	684	46.024	8.349	27.567	1.00 39.05
	ATOM	3695	CD1	TRP	684	47.938	8.374	24.476	1.00 36.48
	ATOM	3696	NE1	TRP	684	46.669	8.720	24.085	1.00 38.70
	ATOM	3697	CZ2	TRP	684	44.483	9.036	25.290	1.00 37.82
	ATOM	3698	CZ3	TRP	684	44.668	8.644	27.664	1.00 38.19
· · · · · · · · · · · · · · · · · · ·	ATOM	3699	CH2	TRP	684	43.918	8.980	26.536	1.00 37.68
	ATOM	3700	С	TRP	684	49.947	6.131	25.020	1.00 31.09
	ATOM	3701	0	TRP	684	49.214	5.332	24.430	1.00 32.25
	ATOM	3702	N	SER	685	50.977	6.750	24.444	1.00 28.90
	MOTA	3703	CA	SER	685	51.345	6.536	23.052	1.00 27.10
	ATOM	3704	СВ	SER	685	52.620	7.312	22.748	1.00 23.88
	ATOM	3705	OG	SER	685	52.459	8.710	22.974	1.00 25.82
	ATOM	3706	С	SER	685	51.567	5.028	22.786	1.00 27.85
	ATOM	3707	0	SER	685	51.172	4.493	21.746	1.00 28.89
	MOTA	3708	N	PHE	686	52.178	4.334	23.741	1.00 28.84
	ATOM	3709	CA	PHE	686	52.410	2.893	23.622	1.00 27.86
	ATOM	3710	CB	PHE	686	53.255	2.403	24.800	1.00 28.14
	ATOM	3711	CG	PHE	686	53.498	0.914	24.803	1.00 28.41
	MOTA	3712	CD1	PHE	686	54.256	0.313	23.802	1.00 27.54
	MOTA	3713	CD2	PHE	686	52.949	0.109	25.796	1.00 29.15
	ATOM	3714	CE1	PHE	686		-1.057	23.792	1.00 24.25
	ATOM	3715	CE2	PHE	686		-1.268	25.790	1.00 27.86
	MOTA	3716	CZ	PHE	686	53.912	-1.850	24.782	1.00 26.09
	MOTA	3717	C	PHE	686	51.072	2.122	23.566	1.00 30.99
	MOTA	3718	0	PHE	686	50.960	1.109	22.873	1.00 29.21
	MOTA	3719	N	GLY	687	50.051	2.603	24.286	1.00 30.57
	ATOM	3720	CA	GLY	687	48.758	1.939	24.273	1.00 31.78
	MOTA	3721	С	GLY	687	48.202	1.923	22.862	1.00 32.51
	MOTA	3722	0	GLY	687	47.687	0.908	22.373	1.00 31.25
	MOTA	3723	N	VAL	688	48.292	3.073	22.204	1.00 32.58
	MOTA	3724	CA	VAL	688	47.825	3.202	20.827	1.00 30.66
	ATOM	3725	CB	VAL	688	47.804	4.684	20.362	1.00 28.55
	ATOM	3726	CG1	VAL	688	47.231	4.795	18.950	1.00 27.25
	ATOM	3727	CG2	VAL	688	46.944	5.522	21.320	1.00 27.12
	ATOM	3728	С	VAL	688	48.684	2.326	19.910	1.00 29.96
	ATOM	3729	0	VAL	688	48.160	1.731	18.974	1.00 30.83
	ATOM	3730	N	LEU	689	49.973	2.202	20.219	1.00 30.02
	ATOM	3731	CA	LEU	689	50.893	1.371	19.430	1.00 30.48
	ATOM	3732	CB	LEU	689	52.359	1.571	19.877	1.00 28.13
	ATOM	3733	CG	LEU	689	53.466	0.966	18.995	1.00 26.34
	ATOM	3734	CD1		689	54.790	1.697	19.174	1.00 25.54
	ATOM	3735	CD2	LEU	689	53.628	-0.505	19.264	1.00 24.99
	ATOM	3736	С	LEU	689	50.479	-0.096	19.567	1.00 30.54
	ATOM	3737	0	LEU	689	50.540		18.602	1.00 27.86
	MOTA	3738	N	LEU	690	50.013	-0.468	20.759	1.00 33.73

ATOM	3739	CA	LEU	690	49.553	-1.830	21.029	1.00 32.47	
ATOM	3740	CB	LEU	690	49.141	-1.982	22.496	1.00 31.82	
ATOM	3741	CG	LEU	690	50.136	-2.220	23.634	1.00 29.71	
ATOM	3742	CD1	LEU	690	49.396	-2.129	24.956	1.00 31.53	
ATOM	3743	CD2	LEU	690	50.771	-3.605	23.483	1.00 31.69	
ATOM	3744	С	LEU	690	48.335	-2.101	20.136	1.00 33.01	
ATOM	3745	0	LEU	690	48.223	-3.168	19.521	1.00 32.68	
ATOM	3746	N	TRP	691	47.423	-1.131	20.089	1.00 32.37	
ATOM	3747	CA	TRP	691	46.230	-1.215	19.256	1.00 32.11	
MOTA	3748	CB	TRP	691	45.424	0.083	19.373	1.00 33.19	
MOTA	3749	CG	TRP	691	44.086	0.055	18.678	1.00 33.95	
MOTA	3750	CD2		691	43.812	0.469	17.337	1.00 30.48	
ATOM	3751		TRP	691	42.434	0.294	17.118	1.00 32.75	
ATOM	3752	CE3		691	44.599	0.989	16.301	1.00 29.47	
ATOM	3753		TRP	691	42.889	-0.352	19.199	1.00 34.34	
ATOM	3754		TRP	691	41.894	-0.211	18.272	1.00 36.53	
ATOM	3755		TRP	691	41.831	0.601	15.900	1.00 30.85	
ATOM	3756		TRP	691	44.003	1.289	15.100	1.00 30.51	
ATOM	3757		TRP	691	42.630	1.104	14.907	1.00 30.29	
ATOM	3758	C	TRP	691	46.661	-1.421	17.805	1.00 31.49	
ATOM	3759	0	TRP	691	46.062	-2.221	17.092	1.00 31.20	
ATOM	3760	N	GLU	692	47.669	-0.656	17.374	1.00 32.90	
ATOM	3761	CA	GLU	692	48.207	-0.734	16.019	1.00 29.78	
ATOM	3762	CB	GLU	692	49.383	0.233	15.809	1.00 25.56	
MOTA	3763	CG	GLU	692	49.009	1.696	15.713	1.00 25.85	
ATOM	3764	CD	GLU	692	50.195	2.570	15.363	1.00 27.76	
ATOM ATOM	3765		GLU	692	51.001	2.850	16.265	1.00 29.52	
ATOM	3766 3767	C C	GLU	692	50.333	2.981	14.191	1.00 26.84	
ATOM	3768	0	GLU GLU	692 692	48.682	-2.136	15.696	1.00 31.08	
ATOM	3769	N	ILE	693	48.545	-2.593	14.553	1.00 32.57	
ATOM	3770	CA	ILE	693	49.774	-2.804 -4.163	16.689	1.00 31.81	
ATOM	3771	СВ	ILE	693	50.666		16.506	1.00 31.87	
ATOM	3772	CG2		693	51.140	-4.614 -6.075	17.699	1.00 33.50	
ATOM	3773	CG1		693	51.879	-3.703	17.513 17.827	1.00 33.06 1.00 34.04	
ATOM	3774	CD1		693	52.744	-4.008	19.025	1.00 34.04	
ATOM	3775	C	ILE	693	48.643	-5.177	16.335	1.00 31.32	
ATOM	3776	0	ILE	693	48.633	-5.982	15.403	1.00 29.55	
MOTA	3777	N	PHE	694	47.654	-5.087	17.207	1.00 33.58	
MOTA	3778	CA	PHE	694	46.550	-6.027	17.178	1.00 36.72	
ATOM	3779	CB	PHE	694	45.980	-6.179	18.589	1.00 36.27	
ATOM	3780	CG	PHE	694	46.988	-6.724	19.547	1.00 34.29	
ATOM	3781	CD1	PHE	694	47.500	-5.949	20.581	1.00 34.95	
ATOM	3782	CD2	PHE	694	47.560	-7.972	19.297	1.00 31.60	
ATOM	3783	CE1	PHE	694	48.576	-6.413	21.344	1.00 35.73	
ATOM	3784	CE2		694	48.633	-8.443	20.049	1.00 31.12	
ATOM	3785		PHE	694	49.149	-7.661	21.066	1.00 33.97	
MOTA	3786	С	PHE	694	45.516	-5.870	16.065	1.00 37.70	
ATOM	3787	0	PHE	694	44.684	-6.756	15.839	1.00 37.99	
MOTA	3788	N	THR	695	45.604	-4.745	15.355	1.00 36.11	
ATOM	3789	CA	THR	695	44.747	-4.485	14.205	1.00 31.23	
ATOM	3790	CB	THR	695	44.107	-3.081	14.236	1.00 30.49	

ATOM	3791	OG1	THR	695	45.133	-2.079	14.134	1.00 30.14		
ATOM	3792	CG2	THR	695	43.329	-2.888	15.512	1.00 31.07		
MOTA	3793	С	THR	695	45.612	-4.619	12.965	1.00 29.79		
MOTA	3794	0	THR	695	45.163	-4.325	11.862	1.00 31.31		
MOTA	3795	N	LEU	696	46.859	-5.051	13.164	1.00 29.75		
ATOM	3796	CA	LEU	696	47.826	-5.259	12.081	1.00 28.46		
ATOM	3797	CB	LEU	696	47.456	-6.495	11.245	1.00 29.96		
ATOM	3798	CG	LEU	696	47.281	-7.848	11.946	1.00 30.38		
ATOM	3799	CD1	LEU	696	47.142	-8.941	10.909	1.00 30.43		
ATOM	3800	CD2	LEU	696	48.46B	-8.138	12.800	1.00 30.45		
ATOM	3801	С	LEU	696	48.101	-4.076	11.160	1.00 32.33		
ATOM	3802	0	LEU	696	48.210	-4.235	9.946	1.00 26.97		
ATOM	3803	N	GLY	697	48.314	-2.900	11.745	1.00 32.70		
MOTA	3804	CA	GLY	697	48.609	-1.705	10.960	1.00 32.70		
ATOM	3805	С	GLY	697	47.432	-0.763	10.817	1.00 32.24		
ATOM	3806	0	GLY	697	47.398	0.099	9.941	1.00 31.81		
ATOM	3807	N	GLY	698	46.455	-0.922	11.700	1.00 32.63		
ATOM	3808	CA	GLY	698	45.277	-0.081	11.643	1.00 31.93		
ATOM	3809	С	GLY	698	45.504	1.411	11.820	1.00 28.95		
ATOM	3810	0	GLY	698	46.454	1.858	12.449	1.00 26.05		
ATOM	3811	N	SER	699	44.569	2.174	11.282	1.00 20.03		
ATOM	3812	CA	SER	699	44.608	3.618	11.352	1.00 30.03		
ATOM	3813	СВ	SER	699	44.095	4.219	10.046	1.00 30.32		
ATOM	3814	OG	SER	699	44.047	5.639	10.095	1.00 33.61		
ATOM	3815	C	SER	699	43.695	4.024	12.492	1.00 30.45		
ATOM	3816	0	SER	699	42.490	3.755	12.450	1.00 29.11		
ATOM	3817	N	PRO	700	44.259	4.591	13.573	1.00 32.27		
ATOM	3818	CD	PRO	700	45.693	4.761	13.881	1.00 29.61		
MOTA	3819	CA	PRO	700	43.408	5.007	14.695	1.00 31.34		
MOTA	3820	CB	PRO	700	44.428	5.358	15.777	1.00 31.30		
ATOM	3821	CG	PRO	700	45.662	5.745	14.989	1.00 29.66		
ATOM	3822	С	PRO	700	42.574	6.208	14.279	1.00 29.65		
MOTA	3823	0	PRO	700	43.032	7.062	13.527	1.00 30.44		
MOTA	3824	N	TYR	701	41.306	6.190	14.660	1.00 30.37		
ATOM	3825	CA	TYR	701	40.359	7.272	14.367	1.00 30.01		
ATOM	3826	CB	TYR	701	40.655	8.474	15.269	1.00 35.19		
ATOM	3827	CG	TYR	701	40.452	8.215	16.749	1.00 39.32		
ATOM	3828	CD1	TYR	701	41.452	8.518	17.675	1.00 43.08		
ATOM	3829	CE1	TYR	701	41.258	8.305	19.041	1.00 46.20		
ATOM	3830	CD2	TYR	701	39.256	7.688	17.229	1.00 40.66		
ATOM	3831	CE2	TYR	701	39.060	7.469	18.584	1.00 43.51		
MOTA	3832	CZ	TYR	701	40.056	7.782	19.485	1.00 45.75		
ATOM	3833	OH	TYR	701	39.847	7.592	20.837	1.00 50.92		
ATOM	3834	С	TYR	701	40.273	7.722	12.909	1.00 29.04		
ATOM	3835	0	TYR	701	40.393	8.904	12.611	1.00 28.53		
ATOM	3836	N	PRO	702	40.015	6.777	11.986	1.00 28.69		
ATOM	3837	CD	PRO	702	39.761	5.346	12.186	1.00 26.94		
ATOM	3838	CA	PRO	702	39.920	7.145	10.569	1.00 27.55		
ATOM	3839	CB	PRO	702	39.709	5.800	9.882	1.00 27.91		
ATOM	3840	CG	PRO	702	39.054	4.971	10.917	1.00 29.04		
ATOM	3841	С	PRO	702	38.790	8.117	10.264	1.00 29.20		
MOTA	3842	0	PRO	702	37.631	7.880	10.617	1.00 32.39		

ATOM	3843	N	GLY	703	39.148	9.213	9.591	1.00 28.34
MOTA	3844	CA	GLY	703	38.191	10.236	9.226	1.00 25.97
ATOM	3845	С	GLY	703	37.960	11.289	10.297	1.00 28.00
ATOM	3846	0	GLY	703	37.175	12.213	10.079	1.00 26.40
ATOM	3847	N	VAL	704	38.621	11.139	11.448	1.00 29.54
ATOM	3848	CA	VAL	704	38.480	12.061	12.576	1.00 30.61
ATOM	3849	CB	VAL	704	38.606	11.324	13.944	1.00 32.54
ATOM	3850	CG1	VAL	704	38.577	12.324	15.111	1.00 31.95
ATOM	3851	CG2	VAL	704	37.482	10.311	14.103	1.00 34.62
MOTA	3852	С	VAL	704	39.490	13.210	12.557	1.00 31.37
MOTA	3853	0	VAL	704	40.683	13.001	12.757	1.00 31.73
MOTA	3854	N	PRO	705	39.030	14.430	12.281	1.00 32.70
ATOM	3855	CD	PRO	705	37.669	14.770	11.819	1.00 33.75
ATOM	3856	CA	PRO	705	39.910	15.599	12.243	1.00 31.90
ATOM	3857	CB	PRO	705	39.065	16.641	11.518	1.00 32.66
ATOM	3858	CG	PRO	705	37.674	16.273	11.906	1.00 35.32
MOTA	3859	С	PRO	705	40.331	16.053	13.635	1.00 31.85
ATOM	3860	0	PRO	705	39.709	15.686	14.634	1.00 31.50
ATOM	3861	N	VAL	706	41.372	16.879	13.676	1.00 32.32
ATOM	3862	CA	VAL	706	41.945	17.389	14.925	1.00 36.88
ATOM	3863	CB	VAL	706	42.991	18.505	14.664	1.00 39.77
MOTA	3864	CG1		706	43.657	18.907	15.974	1.00 39.17
ATOM	3865		VAL	706	44.035	18.057	13.618	1.00 38.70
MOTA	3866	C	VAL	706	40.938	17.923	15.953	1.00 37.80
ATOM	3867	0	VAL	706	40.994	17.581	17.140	1.00 37.45
ATOM	3868	N	GLU	707	39.991	18.724	15.483	1.00 38.19
MOTA	3869	CA	GLU	707	39.009	19.308	16.370	1.00 37.31
ATOM	3870	СВ	GLU	707	38.208	20.361	15.619	1.00 37.46
ATOM	3871	C	GLU	707	38.084	18.264	16.994	1.00 39.56
ATOM	3872	0	GLU	707	37.739	18.344	18.177	1.00 41.39
ATOM ATOM	3873 3874	N CA	GLU	708	37.724	17.260	16.206	1.00 39.99
ATOM	3875	CB	GLU GLU	708 708	36.840	16.212	16.684	1.00 40.08
ATOM	3876	CG	GLU	708 708	36.334	15.377	15.515	1.00 43.96
ATOM	3877	CD	GLU	708	35.505 34.288	16.163 16.851	14.496	1.00 46.61
ATOM	3878	OE1		708	33.659	16.305	15.099 16.040	1.00 52.77
ATOM	3879		GLU	708	33.954	17.955	14.604	1.00 52.52
MOTA	3880	c	GLU	708	37.551	15.337	17.704	1.00 57.04 1.00 39.89
ATOM	3881	0	GLU	708	36.944	14.900	18.684	1.00 39.47
ATOM	3882	N	LEU	709	38.838	15.086	17.471	1.00 39.47
ATOM	3883	CA	LEU	709	39.638	14.277	18.393	1.00 38.33
ATOM	3884	СВ	LEU	709	41.079	14.120	17.892	1.00 34.15
ATOM	3885	CG	LEU	709	42.061	13.338	18.787	1.00 30.94
ATOM	3886	CD1		709	41.861	11.834	18.689	1.00 28.48
ATOM	3887	CD2		709	43.459	13.712	18.395	1.00 29.02
ATOM	3888	С	LEU	709	39.644	14.961	19.751	1.00 25.02
ATOM	3889	0	LEU	709	39.460	14.313	20.787	1.00 38.08
ATOM	3890	N	PHE	710	39.833	16.276	19.749	1.00 39.68
ATOM	3891	CA	PHE	710	39.845	17.021	21.001	1.00 43.27
ATOM	3892	CB	PHE	710	40.024	18.524	20.747	1.00 43.27
ATOM	3893	CG	PHE	710	41.376	18.888	20.225	1.00 46.36
ATOM	3894	CD1		710	42.459	18.024	20.403	1.00 48.33

ATOM	3895		PHE	710	41.579	20.084	19.544	1.00 47.76
ATOM	3896		PHE	710	43.723	18.343	19.915	1.00 51.79
MOTA	3897	CE2		710	42.839	20.417	19.046	1.00 50.36
ATOM	3898	CZ	PHE	710	43.916	19.544	19.233	1.00 53.02
ATOM	3899	С	PHE	710	38.558	16.746	21.758	1.00 44.74
MOTA	3900	0	PHE	710	38.587	16.422	22.952	1.00 44.99
MOTA	3901	N	LYS	711	37.445	16.777	21.032	1.00 45.27
ATOM	3902	CA	LYS	711	36.146	16.529	21.627	1.00 44.00
ATOM	3903	CB	LYS	711	35.031	16.870	20.634	1.00 46.68
ATOM	3904	CG	LYS	711	33.645	16.758	21.235	1.00 52.36
ATOM	3905	CD	LYS	711	32.556	17.224	20.293	1.00 54.43
MOTA	3906,	CE	LYS	711	31.197	16.809	20.826	1.00 55.93
ATOM	3907	NZ	LYS-	711	30.101	17.220	19.912	1.00 63.51
MOTA	3908	С	LYS	711	36.052	15.078	22.120	1.00 42.15
MOTA	3909	0	LYS	711	35.635	14.827	23.250	1.00 40.85
ATOM	3910	N	LEU	712	36.467	14.125	21.294	1.00 40.98
MOTA	3911	CA	LEU	712	36.432	12.719	21.691	1.00 42.26
MOTA	3912	CB	LEU	712	37.012	11.814	20.597	1.00 39.67
MOTA	3913	CG	LEU	712	36.159	11.449	19.381	1.00 39.06
ATOM	3914		LEU	712	36.899	10.440	18.504	1.00 36.97
ATOM	3915		LEU	712	34.842	10.868	19.857	1.00 36.48
ATOM	3916	C	LEU	712	37.232	12.513	22.974	1.00 43.61
ATOM	3917	0	LEU	712	36.796	11.785	23.875	1.00 44.10
ATOM	3918	N	LEU	713	38.407	13.141	23.038	1.00 43.57
ATOM	3919	CA	LEU	713	39.271	13.034	24.207	1.00 43.67
MOTA	3920	CB	LEU	713	40.619	13.726	23.958	1.00 42.24
ATOM	3921	CG	LEU	713	41.569	13.004	22.989	1.00 38.81
ATOM	3922		LEU	713	42.856	13.796	22.817	1.00 30.86
ATOM	3923		LEU	713	41.873	11.591	23.519	1.00 34.27
ATOM	3924	C	LEU	713	38.589	13.594	25.450	1.00 44.78
ATOM	3925	0	LEU	713	38.548	12.919	26.472	1.00 46.04
ATOM	3926	N	LYS	714	38.002	14.785	25.344	1.00 44.72
MOTA	3927	CA	LYS	714	37.304	15.394	26.471	1.00 44.34
MOTA	3928	CB	LYS	714	36.818	16.799	26.114	1.00 43.76
ATOM	3929	CC	LYS	714	37.955	17.761	25.926	1.00 46.37
ATOM	3930	CD	LYS	714	37.497	19.174	25.628	1.00 52.22
MOTA	3931	CE	LYS	714	38.701	20.044	25.235	1.00 57.37
ATOM ATOM	3932	NZ	LYS	714	39.792	20.059	26.279	1.00 58.02
ATOM	3933	C O	LYS	714	36.142	14.534	26.972	1.00 44.17
	3934		LYS	714	35.861	14.499	28.167	1.00 45.14
ATOM ATOM	3935 3936	N	GLU	715	35.498	13.809	26.068	1.00 43.86
ATOM	3937	CA	GLU	715	34.392	12.935	26.430	1.00 42.94
ATOM	3938	CB	GLU	715	33.518	12.652	25.195	1.00 46.57
ATOM		CG	GLU GLU	715	32.930	13.897	24.532	1.00 51.37
ATOM	3939 3940	CD OF 1		715	32.032	13.571	23.338	1.00 54.24
ATOM	3940	OE1 OE2		715	32.215	12.503	22.704	1.00 54.19
ATOM				715	31.139	14.392	23.033	1.00 55.01
ATOM	3942	C	GLU	715	34.878	11.607	27.036	1.00 41.36
	3943	0	GLU	715	34.076	10.730	27.348	1.00 38.24
ATOM	3944	N Cr	GLY	716	36.184	11.452	27.182	1.00 41.41
ATOM	3945	CA	GLY	716	36.727	10.225	27.737	1.00 41.78
ATOM	3946	С	GLY	716	36.602	9.034	26.799	1.00 42.65

ATOM	3947	0	GLY	716	36.661	7.874	27.225	1.00 41.41
ATOM	3948	N	HIS	717	36.439	9.321	25.513	1.00 44.56
ATOM	3949	CA	HIS	717	36.286	8.291	24.502	1.00 45.91
ATOM	3950	CB	HIS	717	35.935	8.926	23.153	1.00 46.65
ATOM	3951	CG	HIS	717	35.860	7.946	22.024	1.00 50.03
MOTA	3952	CD2	HIS	717	34.842	7.171	21.581	1.00 49.92
MOTA	3953	ND1	HIS	717	36.946	7.634	21.235	1.00 51.38
MOTA	3954		HIS	717	36.604	6.708	20.360	1.00 50.10
MOTA	3955	NE2	HIS	717	35.335	6.408	20.550	1.00 49.34
MOTA	3956	C	HIS	717	37.535	7.434	24.354	1.00 47.68
ATOM	3957	0	HIS	717	38.649	7.949	24.287	1.00 49.77
ATOM	3958	N	ARG	718	37.328	6.118	24.283	1.00 48.18
ATOM	3959	CA	ARG	718	38.403	5.148	24.116	1.00 46.95
ATOM	3960	CB	ARG	718	38.571	4.307	25.385	1.00 45.75
ATOM	3961	CG	ARG	718	38.945	5.125	26. 6 18	1.00 47.15
ATOM	3962	CD	ARG	718	40.273	5.852	26.420	1.00 46.61
ATOM	3963	NE	ARG	718	40.722	6.579	27.608	1.00 45.57
ATOM	3964	CZ	ARG	718	40.601	7.896	27.779	1.00 45.48
ATOM	3965		ARG	718	40.033	8.644	26.845	1.00 44.14
ATOM	3966		ARG	718	41.122	8.480	28.854	1.00 43.32
ATOM	3967	С	ARG	718	38.109	4.250	22.912	1.00 47.56
MOTA	3968	0	ARG	718	36.946	3.991	22.589	1.00 48.37
ATOM	3969	N	MET	719	39.149	3.873	22.181	1.00 47.33
ATOM	3970	CA	MET	719	38.984	3.021	21.013	1.00 47.90
ATOM	3971	CB	MET	719	40.282	2.939	20.198	1.00 47.21
ATOM	3972	CG	MET	719	40.652	4.245	19.509	1.00 45.79
ATOM	3973	SD	MET	719	42.095	4.104	18.440	1.00 42.81
ATOM	3974	CE	MET	719	43.377	3.970	19.604	1.00 43.02
ATOM	3975	C	MET	719	38.519	1.629	21.392	1.00 49.99
ATOM	3976	0	MET	719	38.889	1.102	22.450	1.00 47.98
ATOM	3977	N	ASP	720	37.690	1.050	20.523	1.00 53.40
ATOM ATOM	3978 3979	CA	ASP	720	37.135	-0.288	20.722	1.00 53.19
ATOM	3980	CB	ASP ASP	720 720	36.089	-0.638	19.647	1.00 56.95
ATOM	3981		ASP	720 720	34.916	0.333	19.605	1.00 61.65
ATOM	3982		ASP	720	34.908 33.996	1.331	20.356	1.00 68.60
ATOM	3983	C	ASP	720	38.208	0.095	18.792	1.00 61.19
MOTA	3984	o	ASP	720	39.263	-1.372 -1.229	20.713	1.00 51.12 1.00 50.71
ATOM	3985	N	LYS	721	37.926	-2.453	21.432	1.00 48.85
ATOM	3986	CA	LYS	721	38.833	-2.433	21.509	1.00 48.85
ATOM	3987	СВ	LYS	721	38.335	-4.560	22.562	1.00 47.32
ATOM	3988	CG	LYS	721	39.024	-5.901	22.521	1.00 47.79
ATOM	3989	CD	LYS	721	38.493	-6.810	23.597	1.00 51.08
ATOM	3990	CE	LYS	721	38.484	-8.255	23.141	1.00 54.60
MOTA	3991	NZ	LYS	721	38.158	-9.176	24.268	1.00 61.37
ATOM	3992	c	LYS	721	38.861	-4.261	20.155	1.00 49.01
ATOM	3993	0	LYS	721	37.822	-4.688	19.653	1.00 49.01
ATOM	3994	N	PRO	722	40.053	-4.366	19.541	1.00 32.79
ATOM	3995	CD	PRO	722	41.356	-3.839	19.972	1.00 48.92
ATOM	3996	CA	PRO	722	40.167	-5.011	18.233	1.00 46.01
ATOM	3997	СВ	PRO	722	41.663	-4.904	17.918	1.00 45.64
ATOM	3998	CG	PRO	722	42.090	-3.690	18.646	1.00 45.84
				. 	050	3.330	10.010	1.00 1/.00

ATOM	3999	C	PRO	722	39.745	-6.466	18.303	1.00	43.57
MOTA	4000	0	PRO	722	39.719	-7.069	19.381	1.00	41.72
ATOM	4001	N	SER	723	39.360	-7.001	17.150	1.00	43.14
ATOM	4002	CA	SER	723	38.991	-8.398	17.044	1.00	41.85
ATOM	4003	CB	SER	723	38.260	-8.660	15.734	1.00	37.27
MOTA	4004	OG	SER	723	39.112	-8.421	14.639	1.00	39.44
ATOM	4005	C	SER	723	40.339	-9.110	17.049	1.00	41.68
MOTA	4006	0	SER	723	41.299	-8.605	16.493	1.00	40.84
MOTA	4007	N	asn	724	40.405	-10.275	17.683	1.00	45.99
ATOM	4008	CA	ASN	724	41.651	-11.034	17.800	1.00	49.22
MOTA	4009	CB	ASN	724	42.342	-11.215	16.453	1.00	52.35
ATOM	4010	CG	ASN	724	41.768	-12.357	15.668	1.00	58.07
MOTA	4011	ODI	ASN	724	41.821	-13.506	-16.103	1.00	62.42
ATOM	4012	ND2	ASN	724	41.186	-12.054	14.513	1.00	62.13
MOTA	4013	С	ASN	724	42.558	-10.323	18.787	1.00	49.77
ATOM	4014	0	ASN	724	43.698	-9.982	18.494	1.00	51.48
MOTA	4015	N	CYS	725	41.995	-10.054	19.954	1.00	50.34
MOTA	4016	CA	CYS	725	42.698	-9.398	21.028	1.60	49.83
MOTA	4017	CB	CYS	725	42.623	-7.878	20.868	1.00	47.11
MOTA	4018	SG	CYS	725	43.485	-6.992	22.169	1.00	38.55
ATOM	4019	С	CYS	725	42.001	-9.861	22.299	1.00	50.11
ATOM	4020	0	CYS	725	40.772	-9.852	22.383	1.00	50.63
ATOM	4021	N	THR	726	42.788	-10.350	23.244	1.00	50.37
ATOM	4022	CA	THR	726	42.261	-10.843	24.497	1.00	51.05
ATOM	4023	CB	THR	726	43.341	-11.663	25.234	1.00	53.50
ATOM	4024		THR	726	44.292	-10.780	25.829	1.00	57.56
ATOM	4025	CG2	THR	726		-12.554	24.241	1.00	52.55
ATOM	4026	С	THR	726	41.843	-9.665	25.354	1.00	52.18
ATOM	4027	0	THR	726	42.403	-8.574	25.219	1.00	55.14
MOTA	4028	N	ASN	727	40.868	-9.860	26.237	1.00	52.55
ATOM	4029	CA	ASN	727	40.401	-8.781	27.114	1.00	53.17
ATOM	4030	CB	ASN	727	39.246	-9.265	27.992	1.00	60.65
ATOM	4031	CG	ASN	727		-10.545	28.751		68.99
ATOM	4032	OD1		727		-10.718	29.243		73.66
ATOM	4033	ND2		727		-11.454	28.825	1.00	
ATOM	4034	C	ASN	727	41.537	-8.254	27.976		50.79
ATOM ATOM	4035	0	ASN	727	41.513	-7.107	28.414		48.17
ATOM	4036	N Cr	GLU	728	42.527	-9.111	28.215		50.18
ATOM	4037	CA	GLU	728	43.693	-8.764	29.020		49.68
ATOM	4038	CB	GLU	728		-10.011	29.289	1.00	
ATOM	4039	CC	GLU	728		~9.758	30.120	1.00	
ATOM	4040	CD	GLU	728		-11.045	30.542	1.00	
ATOM	4041 4042	OE1		728		-11.930	29.685	1.00	
ATOM	4043	OE2		728		-11.161	31.733	1.00	
ATOM	4044	0	GLU	728	44.509	-7.713	28.272	1.00	
ATOM	4045		GLU	728	44.760	-6.614	28.785	1.00	
ATOM	4045	N CA	LEU	729	44.869	-8.039	27.033	1.00	
ATOM	4046		LEU	729	45.641	-7.137	26.192	1.00	
ATOM	4047	CB CG	LEU	729	45.950	-7.796	24.846	1.00	
ATOM			LEU	729	47.004	-8.900	24.952	1.00	
ATOM	4049	CD1		729	46.960	-9.780	23.749	1.00	
ATOM	4050	CD2	LEU	729	48.404	-8.320	25.139	1.00	33.63

ATOM	4051	C	LEU	729	44.909	-5.817	25.985	1.00 40.58
ATOM	4052	0	LEU	729	45.524	-4.760	25.929	1.00 40.10
MOTA	4053	N	TYR	730	43.591	-5.886	25.917	1.00 39.32
MOTA	4054	CA	TYR	730	42.807	-4.694	25.720	1.00 41.49
ATOM	4055	CB	TYR	730	41.384	-5.052	25.302	1.00 39.70
ATOM	4056	CG	TYR	730	40.507	-3.846	25.099	1.00 39.53
ATOM	4057	CD1	TYR	730	40.828	-2.879	24.142	1.00 35.10
MOTA	4058	CE1	TYR	730	40.019	-1.758	23.958	1.00 36.33
MOTA	4059	CD2	TYR	730	39.352	-3.661	25.874	1.00 38.44
MOTA	4060	CE2	TYR	730	38.537	-2.541	25.696	1.00 37.68
MOTA	4061	CZ	TYR	730	38.876	-1.601	24.730	1.00 36.85
MOTA	4062	OH	TYR	730	38.041	-0.541	24.489	1.00 40.58
ATOM	4063	С	TYR	730	42.814	-3.849	26.993	1.00 43.50
ATOM	4064	0	TYR	730	42.880	-2.621	26.931	1.00 44.45
MOTA	4065	N	MET	731	42.753	-4.492	28.151	1.00 46.53
MOTA	4066	CA	MET	731	42.782	-3.744	29.406	1.00 48.67
MOTA	4067	CB	MET	731	42.488	-4.668	30.590	1.00 54.90
MOTA	4068	CG	MET	731	41.072	-5.229	30.577	1.00 63.75
MOTA	4069	SD	MET	731	39.766	-3.998	30.763	1.00 69.82
MOTA	4070	CE	MET	731	39.849	-3.788	32.581	1.00 68.20
ATOM	4071	С	MET	731	44.148	-3.087	29.551	1.00 45.73
ATOM	4072	0	MET	731	44.273	-2.024	30.160	1.00 42.09
MOTA	4073	N	MET	732	45.168	-3.728	28.986	1.00 43.47
MOTA	4074	CA	MET	732	46.519	-3.189	29.024	1.00 43.85
ATOM	4075	CB	MET	732	47.515	-4.154	28.365	1.00 40.67
ATOM	4076	CG	MET	732	48.966	-3.646	28.369	1.00 39.96
ATOM	4077	SD	MET	732	50.252	-4.870	27.887	1.00 35.34
ATOM	4078	CE	MET	732	50.523	-5. 6 67	29.390	1.00 35.15
ATOM	4079	С	MET	732	46.460	-1.860	28.275	1.00 43.91
MOTA	4080	0	MET	732	46.924	-0.835	28.782	1.00 47.29
MOTA	4081	N	MET	733	45.798	-1.860	27.120	1.00 42.51
ATOM	4082	CA	MET	733	45.639	-0.652	26.319	1.00 39.85
MOTA	4083	CB	MET	733	44.888	-0.932	25.013	1.00 38.08
ATOM	4084	CG	MET	733	45.614	-1.805	23.991	1.00 37.14
ATOM	4085	SD	MET	733	44.509	-2.170	22.578	1.00 37.32
ATOM	4086	CE	MET	733	45.198	-3.684	21.929	1.00 28.98
ATOM	4087	С	MET	733	44.838	0.363	27.123	1.00 41.12
ATOM	4088	0	MET	733	45.228	1.532	27.213	1.00 44.38
ATOM	4089	N	ARG	734	43.737	-0.084	27.731	1.00 40.28
ATOM	4090	CA	ARG	734	42.893	0.813	28.516	1.00 40.23
ATOM	4091	СВ	ARG	734	41.632	0.095	29.007	1.00 39.95
ATOM	4092	CG	ARG	734	40.723	-0.384	27.894	1.00 36.41
ATOM	4093	CD	ARG	734	40.323	0.741	26.995	1.00 39.31
ATOM	4094	NE	ARG	734	39.510	1.733	27.682	1.00 48.97
ATOM	4095	CZ	ARG	734	38.182	1.681	27.774	1.00 53.99
ATOM	4096	NH1		734	37.503	0.681	27.222	1.00 56.64
ATOM	4097	NH2		734	37.526	2.633	28.416	1.00 56.79
MOTA	4098	С	ARG	734	43.694	1.387	29.675	1.00 39.38
ATOM	4099	0	ARG	734	43.538	2.564	30.010	1.00 41.82
ATOM	4100	N	ASP	735	44.583	0.572	30.244	1.00 37.67
MOTA	4101	CA	ASP	735	45.465	1.000	31.339	1.00 39.58
ATOM	4102	CB	ASP	735	46.392	-0.137	31.773	1.00 42.90

ATOM 4103 CG ASP 735 45.690 -1.175 32.604 1.00 47.78 MOTA 4104 OD1 ASP 735 46.116 -2.355 32.524 1.00 47.92 MOTA 4105 OD2 ASP 735 44.733 -0.803 33.339 1.00 46.75 MOTA 4106 С ASP 735 46.339 2.161 30.881 1.00 37.68 **ATOM** 4107 0 ASP 735 46.447 3.178 31.579 1.00 36.83 **ATOM** 4108 N CYS 736 46.996 1.967 29.734 1.00 35.06 **MOTA** 4109 CA CYS 736 47.858 2.979 29.140 1.00 32.91 ATOM 4110 CB CYS 736 48.499 2.469 27.848 1.00 27.65 MOTA 4111 SG CYS 736 49.631 1.067 27.989 1.00 31.08 MOTA 4112 С CYS 736 47.054 4.232 28.828 1.00 35.28 ATOM 4113 0 CYS 736 47.595 5.334 28.810 1.00 35.52 MOTA 4114 N TRP 737 45.742 4.078 28.677 1.00 38.73 MOTA 4115 CA TRP 737 · 44.885 5.217 28.352 1.00 41.10 **ATOM** 4116 CB TRP 737 43.890 4.816 27.266 1.00 41.22 **ATOM** 4117 CG TRP 737 44.535 4.362 25.994 1.00 40.65 ATOM 4118 CD2 TRP 737 43.976 3.465 25.026 1.00 41.90 ATOM 4119 CE2 TRP 737 44.932 3.325 23.990 1.00 41.02 **ATOM** 4120 CE3 TRP 737 42.763 2.764 24.930 1.00 40.44 **ATOM** 4121 CD1 TRP 737 45.766 4.721 25.517 1.00 39.14 **ATOM** 4122 NEI TRP 737 46.011 4.103 24.316 1.00 37.93 **MOTA** 4123 CZ2 TRP 737 44.708 2.512 22.875 1.00 40.92 ATOM 4124 CZ3 TRP 737 42.549 1.956 23.820 1.00 38.42 **ATOM** 4125 CH2 TRP 737 43.518 1.837 22.812 1.00 36.49 **ATOM** 4126 С TRP 737 44.159 5.847 29.538 1.00 41.39 **ATOM** 4127 0 TRP 737 43.163 6.551 29.366 1.00 40.86 MOTA 4128 N HIS 738 44.685 5.643 30.743 1.00 43.61 MOTA 4129 CA HIS 738 44.059 6.197 31.941 1.00 44.35 MOTA 4130 CB HIS 738 44.698 5.596 33.183 1.00 45.31 **ATOM** 4131 CG HIS 738 5.922 34.446 43.970 1.00 50.87 ATOM 4132 CD2 HIS 738 43.685 7.111 35.026 1.00 49.13 MOTA 4133 ND1 HIS 738 43.401 4.961 35.252 1.00 52.48 ATOM 4134 CE1 HIS 738 42.798 5.541 36.275 1.00 55.70 MOTA 4135 NE2 HIS 738 42.955 6.848 36.159 1.00 51.42 MOTA 4136 С HIS 738 44.202 7.714 31.969 1.00 44.15 MOTA 4137 0 HIS 738 45.294 8.223 31.787 1.00 43.14 MOTA 4138 N **ALA** 739 43.115 8.428 32.272 1.00 45.42 MOTA 4139 CA ALA 739 32.318 1.00 47.29 43.141 9.895 MOTA 4140 CB ALA 739 41.792 10.426 32.752 1.00 49.75 MOTA 4141 C ALA 739 44.240 33.223 1.00 48.73 10.454 MOTA 4142 0 ALA 739 44.921 11.415 32.868 1.00 49.32 MOTA 4143 N VAL 740 44.331 9.893 34.425 1.00 50.51 MOTA 4144 CA VAL 740 45.332 10.262 35.424 1.00 51.32 MOTA 4145 CB VAL 740 44.861 9.880 36.842 1.00 52.29 MOTA 4146 CG1 VAL 740 45.905 10.254 37.869 1.00 53.73 **MOTA** 4147 CG2 VAL 740 43.551 10.575 37.152 1.00 53.54 ATOM 4148 С VAL 740 46.656 9.535 35.121 1.00 51.06 ATOM 4149 0 VAL 740 46.780 8.320 35.348 1.00 50.81 MOTA 4150 N PRO 741 47.670 10.280 34.657 1.00 50.12 MOTA 4151 CD PRO 741 47.595 34.454 11.738 1.00 50.19 **ATOM** 4152 CA PRO 741 49.003 9.775 34.294 1.00 51.10 ATOM 4153 CB PRO 741 49.790 11.060 34.024 1.00 50.35 MOTA CG PRO 4154 741 48.731 11.978 33.492 1.00 50.13

MOTA	4155	С	PRO	741	49.687	8.902	35.340	1.00 52.02
MOTA	4156	0	PRO	741	50.374	7.941	34.998	1.00 50.79
MOTA	4157	N	SER	742	49.482	9.228	36.613	1.00 53.75
ATOM	4158	CA	SER	742	50.079	8.474	37.708	1.00 54.58
ATOM	4159	CB	SER	742	49.921	9.245	39.020	1.00 57.25
ATOM	4160	OG	SER	742	48.572	9.629	39.237	1.00 61.69
MOTA	4161	C	SER	742	49.479	7.077	37.851	1.00 53.33
MOTA	4162	О	SER	742	50.074	6.189	38.464	1.00 52.98
MOTA	4163	N	GLN	743	48.286	6.897	37.305	1.00 52.97
MOTA	4164	CA	GLN	743	47.616	5.613	37.390	1.00 52.15
MOTA	4165	CB	GLN	743	46.108	5.827	37.505	1.00 56.12
ATOM	4166	CG	GLN	743	45.506	5.374	38.838	1.00 60.50
ATOM	4167	_ CD .	GLN	743	46.269	5.887	40.046	1.00 64.45
MOTA	4168	OE1		743	46.910	5.114	40.752	1.00 65.64
ATOM	4169	NE2	GLN	743	46.199	7.194	40.290	1.00 67.99
MOTA	4170	C	GLN	743	47.963	4.690	36.229	1.00 49.54
ATOM	4171	0	GLN	743	47.629	3.499	36.246	1.00 50.07
MOTA	4172	N	ARG	744	48.605	5.241	35.202	1.00 46.93
ATOM	4173	CA	ARG	744	49.010	4.437	34.044	1.00 44.51
ATOM	4174	CB	ARG	744	49.478	5.330	32.894	1.00 39.30
ATOM	4175	CG	ARG	744	48.433	6.300	32.360	1.00 32.53
ATOM	4176	CD	ARG	744	48.991	7.178	31.254	1.00 25.50
ATOM	4177	NE	ARG	744	48.034	8.218	30.932	1.00 32.16
ATOM	4178	CZ	ARG	744	48.352	9.454	30.542	1.00 34.35
ATOM	4179	NH1		744	49.622	9.814	39.40C	1.00 30.49
ATOM ATOM	4180		ARG	744	47.382	10.349	30.350	1.00 32.23
ATOM	4181 4182	С О	ARG	744	50.153	3.498	34.472	1.00 44.61
ATOM	4183	N	ARG	744	50.833	3.741	35.474	1.00 47.68
ATOM	4184	CD	PRO PRO	745	50.319	2.365	33.765	1.00 43.21
ATOM	4185	CA	PRO	745 245	49.444	1.737	32.763	1.00 42.00
ATOM	4186	CB	PRO	745 745	51.414	1.470	34.157	1.00 40.11
ATOM	4187	CG	PRO	745	51.004 50.251	0.132	33.532	1.00 37.54
ATOM	4188	C	PRO	745	52.744	0.515 1.956	32.335	1.00 36.49
ATOM	4189	ō	PRO	745	52.807	2.654	33.612 32.602	1.00 39.15
ATOM	4190	N	THR	746	53.812	1.626	34.316	1.00 40.56
ATOM	4191	CA	THR	746	55.135	2.020	33.886	1.00 37.77 1.00 37.61
ATOM	4192	СВ	THR	746	56.113	2.132	35.000	1.00 39.14
ATOM	4193	OG1	THR	746	56.439	0.824	35.600	1.00 35.14
MOTA	4194	CG2	THR	746	55.489	2.990	36.195	1.00 36.82
MOTA	4195	С	THR	746	55.687	1.036	32.852	1.00 36.75
ATOM	4196	0	THR	746	55.228	-0.103	32.772	1.00 32.89
ATOM	4197	N	PHE	747	56.649	1.482	32.043	1.00 36.56
MOTA	4198	CA	PHE	747	57.267	0.599	31.055	1.00 33.79
ATOM	4199	СВ	PHE	747	58.305	1.350	30.226	1.00 28.85
ATOM	4200	CG	PHE	747	57.702	2.123	29.103	1.00 30.71
ATOM	4201	CD1		747	57.060	1.455	28.059	1.00 26.42
ATOM	4202	CD2		747	57.749	3.510	29.080	1.00 28.73
ATOM	4203	CE1		747	56.469	2.154	27.025	1.00 26.56
MOTA	4204			747	57.150	4.216	28.047	1.00 28.97
ATOM	4205	CZ	PHE	747	56.518	3.535	27.018	1.00 28 95
ATOM	4206	C	PHE	747	57.901	-0.593	31.732	1.00 34.64
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ATOM	4207	0	PHE	747	58.008	-1.667	31.156	1.00 31.47
ATOM	4208	N	LYS	748	58.328	-0.399	32.972	1.00 38.86
MOTA	4209	CA	LYS	748	58.920	-1.480	33.727	1.00 39.79
ATOM	4210	CB	LYS	748	59.529	-0.952	35.026	1.00 43.68
MOTA	4211	CG	LYS	748	60.200	-2.047	35.838	1.00 48.11
MOTA	4212	CD	LYS	74B	60.917	-1.515	37.064	1.00 51.33
ATOM	4213	CE	LYS	748	61.353	-2.660	37.973	1.00 51.17
MOTA	4214	NZ	LYS	748	62.135	-2.141	39.127	1.00 56.55
ATOM	4215	С	LYS	748	57.813	-2.503	34.008	1.00 41.14
ATOM	4216	0	LYS	748	58.025	-3.706	33.848	1.00 38.24
ATOM	4217	N	GLN	749	56.622	-2.008	34.383	1.00 41.20
ATOM	4218	CA	GLN	749	55.454	-2.856	34.669	1.00 40.49
MOTA	4219	CB	GLN	749	54.254	-2.015	35.134	1.00 45.70
ATOM	4220	CG	GLN	749	54.378	-1.368	36.500	1.00 50.61
MOTA	4221	CD	GLN	749	53.203	-0.441	36.797	1.00 55.26
ATOM	4222	OE1		749	53.392	0.727	37.123	1.00 58.00
ATOM	4223	NE2		749	51.988	-0.951	36.665	1.00 59.25
ATOM	4224	С	GLN	749	55.049	-3.588	33.397	1.00 37.42
ATOM	4225	0	GLN	749	54.964	-4.810	33.369	1.00 36.00
ATOM	4226	N	LEU	750	54.810	-2.817	32.340	1.00 36.76
ATOM	4227	CA	LEU	750	54.409	-3.355	31.033	1.00 35.39
ATOM	4228	CB	LEU	750	54.358	-2.241	29.984	1.00 30.97
ATOM	4229	CG	LEU	750	53.369	-1.091	30.177	1.00 27.36
MOTA	4230		LEU	750	53.745	0.037	29.217	1.00 29.15
ATOM ATOM	4231		TEU	750	51.941	-1.578	29.934	1.00 29.22
	4232	C	LEU	750	55.369	-4.437	30.557	1.00 35.16
ATOM ATOM	4233	0	LEU	750	54.934	-5.449	30.014	1.00 34.45
ATOM	4234	N	VAL	751 751	56.673	-4.212	30.721	1.00 38.76
ATOM	4235 4236	CA	VAL	751	57.656	-5.217	30.312	1.00 38.69
ATOM	4237	CB	VAL VAL	751	59.129	-4.724	30.485	1.00 33.81
ATOM	4238	CG2		751 751	60.092	-5.836	30.120	1.00 32.04
ATOM	4239	C	VAL	751 751	59.415	-3.535	29.598	1.00 30.67
ATOM	4240	0	VAL	751 751	57.428	-6.493	31.131	1.00 41.68
ATOM	4241	N	GLU	752	57.492 57.109	-7.599	30.594	1.00 39.92
ATOM	4242	CA	GLU	752 752	56.854	-6.338 -7.501	32.414	1.00 44.22
ATOM	4243	СВ	GLU	752 752	56.779	-7.078	33.266 34.743	1.00 47.43 1.00 49.29
ATOM	4244	CG	GLU	752	58.093	-6.448	35.212	1.00 49.29
ATOM	4245	CD	GLU	752	58.215	-6.249	36.707	1.00 53.35
ATOM	4246		GLU	752	58.554	-5.123	37.136	1.00 53.63
ATOM	4247		GLU	752	58.021	-7.228	37.452	1.00 56.18
ATOM	4248	С	GLU	752	55.594	-8.256	32.809	1.00 46.90
ATOM	4249	0	GLU	752	55.646	-9.464	32.551	1.00 43.85
ATOM	4250	N	ASP	753	54.490	-7.529	32.640	1.00 48.05
ATOM	4251	CA	ASP	753	53.232	-8.128	32.193	1.00 48.46
MOTA	4252	СВ	ASP	753	52.119	-7.090	32.118	1.00 51.25
MOTA	4253	CG	ASP	753	51.579	-6.707	33.467	1.00 54.20
MOTA	4254		ASP	753	51.440	-7.589	34.330	1.00 57.31
ATOM	4255		ASP	753	51.281	-5.513	33.659	1.00 55.58
MOTA	4256	С	ASP	753	53.371	-8.771	30.837	1.00 48.59
MOTA	4257	0	ASP	753	53.001	-9.930	30.649	1.00 49.69
MOTA	4258	N	LEU	754	53.903	-8.009	29.889	1.00 47.21
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MOTA	4259	CA	LEU	754	54.102 -8	.489 28.523	1.00 46.37
MOTA	4260	CB	LEU	754	54.664 -7	.385 27.625	1.00 44.16
MOTA	4261	CG	LEU	754	53.621 -6	.366 27.152	1.00 46.35
MOTA	4262	CD1	LEU	754	54.296 -5	.272 26.343	1.00 45.11
ATOM	4263	CD2	LEU	754	52.514 -7	.070 26.349	1.00 42.89
ATOM	4264	C	LEU	754	55.004 -9	.703 28.481	1.00 47.08
ATOM	4265	0	LEU	754	54.818 -10	.590 27.659	1.00 45.02
ATOM	4266	N	ASP	755	55.969 -9	.755 29.385	1.00 49.68
ATOM	4267	CA	ASP	755	56.890 -10	.876 29.487	1.00 51.62
ATOM	4268	CB	ASP	755	57.883 -10	.586 30.615	1.00 54.90
ATOM	4269	CG	ASP	755	59.009 -11	.589 30.702	1.00 59.00
ATOM	4270	OD1	ASP	755 ·	59.694 -11	.608 31.746	1.00 63.70
ATOM	4271	OD2	ASP	755	59.223 -12	346 29.728	1.00 60.31
MOTA	4272	С	ASP	755	56.059 -12	.117 29.817	1.00 51.50
MOTA	4273	0	ASP	755	56.119 <i>-</i> 13.	150 29.138	1.00 47.11
MOTA	4274	N	ARG	756	55.237 -11.		1.00 51.81
ATOM	4275	CA	ARG	756	54.362 -13	009 31.328	1.00 51.44
MOTA	4276	CB	ARG	756	53.635 -12.	519 32.582	1.00 54.52
ATOM	4277	CG	ARG	756	52.459 -13.	358 33.027	1.00 55.00
ATOM	4278	CD	ARG	756	51.815 -12.	727 34.255	1.00 59.54
ATOM	4279	NE	ARG	756	51.417 -11.	335 34.026	1.00 64.01
ATOM	4280	CZ	ARG	756	50.366 -10.	960 33.301	1.00 65.76
MOTA	4281	NH1	ARG	756	49.598 -11.	866 32.721	1.00 63.56
ATOM	4282	NH2	ARG	756	50.061 -9.	676 33.183	1.00 66.59
MOTA	4283	C	ARG	756	53.361 -13.	440 30.260	1.00 50.03
MOTA	4284	0	ARG	756	53.267 -14.	622 29.960	1.00 49.98
ATOM	4285	N	ILE	757	52.645 -12.	483 29.673	1.00 46.87
MOTA	4286	CA	ILE	757	51.656 -12.	789 28.644	1.00 44.28
MOTA	4287	CB	ILE	757	50.919 -11.	532 28.125	1.00 40.46
MOTA	4288		ILE	757	49.923 -11.	923 27.062	1.00 38.44
ATOM	4289	CG1	ILE	757	50.202 -10.	830 29.277	1.00 39.74
MOTA	4290	CD1	ILE	757	49.481 -9.	551 28.920	1.00 40.68
ATOM	4291	С	ILE	757	52.251 -13.	528 27.454	1.00 44.20
MOTA	4292	0	ILE	757	51.643 -14.	469 26.959	1.00 40.28
ATOM	4293	N	VAL	758	53.440 -13.	111 27.014	1.00 47.56
ATOM	4294	CA	VAL	758	54.102 -13.	745 25.874	1.00 48.90
ATOM	4295	CB	VAL	758	55.543 -13.		1.00 47.01
ATOM	4296	CG1		758	56.198 -13.	920 24.456	1.00 44.38
ATOM	4297	CG2		758	55.493 -11.		1.00 47.85
ATOM	4298	С	VAL	758	54.249 -15.		1.00 51.79
ATOM	4299		VAL	758	54.043 -16.		1.00 49.80
MOTA	4300	N	ALA	759	54.622 -15.		1.00 54.80
ATOM	4301	CA	ALA	759	54.825 -16.		1.00 57.15
ATOM	4302		ALA	759	55.406 -16.		1.00 56.77
ATOM	4303		ALA	759	53.524 -17.		1.00 60.83
ATOM	4304		ALA	759	53.487 -18.		1.00 63.59
ATOM	4305		LEU	760	52.452 -17.		1.00 61.74
ATOM	4306		LEU	760	51.151 -17.		1.00 61.29
ATOM	4307		LEU	760	50.280 -17.		1.00 60.41
ATOM	4308		LEU	760	50.808 -17.		1.00 58.68
ATOM	4309	CD1		760	49.917 -16.		1.00 59.64
ATOM	4310	CD2	LEU	760	50.899 -18.	799 31.138	1.00 57.84

ATOM	4311	С	LEU	760	50.439	-17.706	26.951	1.00 63.42
ATOM	4312	0	LEU	760	49.282	-18.121	26.842	1.00 63.68
ATOM	4313	N	THR	761	51.113	-17.200	25.924	1.00 66.71
ATOM	4314	CA	THR	761	50.512	-17.109	24.586	1.00 68.48
MOTA	4315	CB	THR	761	50.794	-15.734	23.922	1.00 68.21
MOTA	4316	OG1	THR	761	50.193	-14.695	24.701	1.00 70.34
MOTA	4317	CG2	THR	761	50.202	-15.684	22.530	1.00 64.45
ATOM	4318	С	THR	761	51.030	-18.225	23.688	1.00 69.65
ATOM	4319	0	THR	761	52.230	-18.492	23.623	1.00 70.43
MOTA	4320	SG	CYS	1603	18.668	-9.074	20.131	0.50 30.57
MOTA	4321	CG	MET	534	69.414	12.079	23.224	0.50 36.86
MOTA	4322	SD	MET	534	69.162	13.149	24.646	0.50 40.20
MOTA	·- 4323	CE	MET	534	70.204	12.299	25.912	0.50 41.95
ATOM	4324	SG	CYS	603	56.218	-8.072	16.341	0.50 37.35
ATOM	4325	OH2	TIP	1	71.863	25.340	2.719	1.00 24.40
MOTA	4326	OH2	TIP	2	39.671	4.177	15.837	1.00 36.87
ATOM	4327	OH2	TIP	3	83.765	19.802	10.549	1.00 26.81
ATOM	4328	OH2	TIP	4	83.844	20.193	7.757	1.00 30.07
MOTA	4329	OH2	TIP	5	75.192	16.430	6.693	1.00 26.76
MOTA	4330	OH2	TIP	6	86.579	19.662	9.323	1.00 36.11
MOTA	4331	OH2	TIP	7	52.204	10.911	24.392	1.00 36.83
ATOM	4332	OH2	TIP	8	55.174	9.435	22.514	1.00 21.93
MOTA	4333	OH2	TIP	9	57.077	4.556	32.580	1.00 25.17
ATOM	4334	OH2	TIP	10	52.281	4.737	13.300	1.00 20.79
MOTA	4335	OH2	TIP	11	41.402	5.304	22.893	1.00 39.17
MOTA	4336	OH2	TIP	12	45.088	8.857	21.604	1.00 35.14
MOTA	4337	OH2		13	64.519	-2.772	28.799	1.00 47.52
MOTA	4338	OH2	TIP	14	77.327	12.960	23.832	1.00 34.47
ATOM	4339	OH2		15	79.366	17.021	18.247	1.00 47.49
ATOM	4340		TIP	16	83.087	11.573	15.986	1.00 22.80
MOTA	4341		TIP	17	13.977	-9.804	0.222	1.00 24.88
ATOM	4342		TIP	18	38.451	0.155	5.081	1.00 41.03
ATOM	4343		TIP	20	27.109	6.286	4.902	1.00 27.69
ATOM	4344		TIP	21	34.379	-1.750	16.771	1.00 47.69
ATOM	4345		TIP	22	20.394	2.449	27.821	1.00 54.32
ATOM	4346	OH2	TIP	23		-11.642	38.062	1.00 45.31
MOTA	4347	OH2	TIP	24	17.137	-5.949	-1.716	1.00 27.63
ATOM	4348		TIP	25	27.604	7.961	15.119	1.00 47.19
ATOM	4349		TIP	26	31.446	0.136	6.605	1.00 29.98
ATOM	4350	OH2		27		-13.047	27.803	1.00 28.86
ATOM	4351	OH2		28		-17.191	13.067	1.00 37.44
MOTA	4352	OH2		29	88.748	14.279	8.091	1.00 32.72
ATOM	4353	OH2		30	-2.392	-3.684	11.343	1.00 41.86
MOTA	4354	OH2		31	34.968	-4.221	18.549	1.00 40.51
ATOM	4355	OH2		32	80.581	17.982	9.655	1.00 27.85
ATOM	4356	OH2		33	5.522	3.773	10.805	1.00 24.60
ATOM	4357	OH2		34	-10.747	5.416	11.174	1.00 29.27
ATOM	4358	OH2		35	29.049	-8.816	19.978	1.00 35.24
ATOM	4359	OH2		36	5.871	3.463	13.481	1.00 26.62
ATOM	4360	OH2		37	31.834	2.899	0.207	1.00 49.70
MOTA	4361	OH2		38	19.799	2.012	-3.941	1.00 29.67
MOTA	4362	OH2	TIP	39	62.060	2.679	32.659	1.00 54.86

MOTA	4363	OH2	TIP	40	21.100	-6.883	-4.054	1.00 22.33
MOTA	4364	OH2	TIP	41	-15.675	8.744	22.559	1.00 44.54
ATOM	4365	OH2	TIP	42	40.066	2.225	8.567	1.00 57.00
MOTA	4366	OH2	TIP	43	19.477	11.293	-0.049	1.00 37.77
ATOM	4367	OH2	TIP	44	67.060	9.047	17.334	1.00 25.14
ATOM	4368	OH2	TIP	45	87.829	18.937	18.529	1.00 45.92
MOTA	4369	OH2	TIP	46	74.741	16.956	3.987	1.00 40.33
ATOM	4370	OH2	TIP	47	29.411		10.525	1.00 38.41
ATOM	4371	OH2	TIP	48	66.592	7.020	15.108	1.00 36.15
MOTA	4372	OH2	TIP	49	85.071		5.755	1.00 19.89
ATOM	4373	OH2	TIP	50	-4.842		3.118	1.00 28.22
ATOM	4374	OH2	TIP	51	19.454	5.250	4.876	1.00 34.86
MOTA	_4375.	OH2	TIP	53	34.785	5.433	24.743	1.00 30.40
ATOM	4376	OH2	TIP	54	34.792	-17.150	13.665	1.00 35.81
ATOM	4377	OH2	TIP	55	59.956	7.380	27.941	1.00 36.76
ATOM	4378	OH2	TIP	56	-7.327	-1.518	6.428	1.00 39.13
MOTA	4379	OH2	TIP	57	55.164	12.120	25.338	1.00 38.87
ATOM	4380	OH2	TIP	58	68.637	6.832	16.698	1.00 54.96
MOTA	4381	OH2		59	73.778	20.869	19.031	1.00 35.01
ATOM	4382	OH2	TIP	60	3.582	-8.363	-8.103	1.00 16.71
ATOM	4383	OH2	TIP	61	38.051	10.933	5.487	1.00 32.85
ATOM	4384	OH2		62	29.727	-9.630	-1.370	1.00 30.92
ATOM	4385	OH2	TIP	64	49.186	1.253	12.066	1.00 42.67
MOTA	4386	OH2	TIP	65	41.375	3.989	28.951	1.00 37.95
ATOM	4387	OH2	TIP	66	10.798	-13.119	1.125	1.00 38.26
MOTA	4388	OH2	TIP	67	-1.079	-4.386	21.428	1.00 27.92
ATOM	4389	OH2	TIP	68	30.327	16.346	13.295	1.00 53.21
ATOM	4390	OH2	TIP	69	8.319	4.437	3.449	1.00 23.63
MOTA	4391	OH2	TIP	70	73.152	18.809	22.631	1.00 36.45
ATOM	4392	OH2	TIP	7 1	-7.984	-3.476	25.048	1.00 33.16
MOTA	4393	OH2	TIP	72	66.529	-4.720	28.421	1.00 66.32
ATOM	4394	OH2	TIP	73		-20.723	4.868	1.00 48.14
ATOM	4395	OH2	TIP	74	59.417	-6.760	4.957	1.00 48.73
ATOM	4396	OH2	TIP	75	16.509	-13.306	-2.942	1.00 41.02
ATOM	4397	OH2	TIP	76	-15.064	7.473	4.275	1.00 26.77
ATOM	4398	OH2	TIP	77	33.118	2.917	13.384	1.00 41.38
ATOM	4399	OH2	TIP	78	0.112	-2.913	10.809	1.00 27.49
MOTA	4400	OH2	TIP	79	17.448	2.562	5.507	1.00 16.32
ATOM	4401	OH2	TIP	81	27.445	3.796	6.134	1.00 29.83
MOTA	4402	OH2	TIP	82	-8.708	6.231	9.598	1.00 27.66
MOTA	4403	OH2	TIP	83	1.565	-1.998	8.758	1.00 33.46
MOTA	4404	OH2	TIP	84	-4.774	-3.153	7.049	1.00 36.59
ATOM	4405	OH2	TIP	85	17.443	3.105	1.795	1.00 20.39
MOTA	4406	OH2	r IP	86	20.120	3.387	2.918	1.00 30.35
MOTA	4407	OH2	rip	87	0.466	-2.238	22.190	1.00 20.30
ATOM	4408	OH2	rip	88	19.749	-6.018	-1.687	1.00 21.33
MOTA	4409	ОН2		89		-15.695	6.861	1.00 38.80
ATOM	4410	OH2	rip	90		-12.113	11.774	1.00 34.18
MOTA	4411	ОН2 7		91	6.297	1.090	-3.192	1.00 24.40
ATOM	4412	он2 1	rip	92	-13.540	1.554	5.413	1.00 34.94
ATOM	4413	ОН2 1	rip	93	15.607	-7.315	0.017	1.00 26.30
ATOM	4414	OH2 T		94	-1.868	-5.461	3.839	1.00 37.12
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ATOM	4415	OH	? TIP	95	12.718	5.095	-4.401	1.00 40.61
ATOM	4416	OH	? TIP	96	69.849	27.233	2.056	1.00 41.42
ATOM	4417	OH	? TIP	97	24.374	-13.311	0.143	1.00 52.75
ATOM	4418		? TIP	98	60.424	-4.582	34.237	1.00 42.02
ATOM	4419		TIP	99	10.589	5.757	3.485	1.00 61.53
MOTA	4420		TIP	100	-9.564	-3.999	4.718	1.00 29.02
MOTA	4421	OH2	TIP	101	73.085	-1.967	10.565	1.00 59.23
ATOM	4422	OH2	TIP	102	-3.172	5.701	30.623	1.00 30.51
MOTA	4423	OH2	TIP	103	36.672	0.620	11.780	1.00 53.77
ATOM	4424	OH2	TIP	104	21.408	6.462	16.955	1.00 27.62
MOTA	4425	OH2		105	31.224	0.791	19.345	1.00 77.65
ATOM '	4426		TIP	106	5.660	-8.451	22.197	1.00 49.50
ATOM	4427	OH2	TIP	107 -	-12.988	8.471	17.441	1.00 31.69
ATOM	4428	OH2	TIP	108	26.733	-10.524	-0.894	1.00 25.26
MOTA	4429	OH2		109	24.182	2.026	18.156	1.00 35.87
MOTA	4430	OH2	TIP	110	-1.822	12.848	3.561	1.00 35.44
ATOM	4431	OH2		111	59.584	13.491	33.225	1.00 40.47
ATOM	4432		TIP	112	4.402	-10.813	1.929	1.00 47.07
ATOM	4433		TIP	113	8.032	2.916	0.940	1.00 40.79
ATOM	4434		TIP	114	75.905	1.522	25.912	1.00 55.51
ATOM	4435		TIP	115	48.960	15.737	14.249	1.00 38.97
ATOM	4436		TIP	116	2.333	-11.271	9.174	1.00 29.12
ATOM	4437		TIP	117	83.062	26.404	12.925	1.00 41.17
ATOM	4438		TIP	118	8.816	-6.440	-3.424	1.00 48.26
ATOM	4439		TIP	119	-8.594	4.575	4.258	1.00 32.68
ATOM	4440	OH2		120	7.695	-13.769	8.401	1.00 39.22
ATOM	4441	OH2		121	51.500	6.285	10.369	1.00 25.18
ATOM	4442		TIP	122	20.720	3.849	15.625	1.00 22.46
ATOM	4443		TIP	123	73.111	3.718	20.617	1.00 28.26
ATOM	4444	OH2	TIP	124	5.312	-11.608	22.516	1.00 32.74
ATOM	4445		TIP	125	34.207	2.437	16.601	1.00 65.04
ATOM	4446		TIP	126		-11.998	7.085	1.00 25.13
ATOM	4447			127	B.227	3.912	-1.495	1.00 43.73
ATOM	4448		TIP	129	7.312	7.072	2.922	1.00 47.65
ATOM	4449		TIP	130	35.824	-1.660	0.135	1.00 30.43
ATOM	4450		TIP	131	44.723	10.285	11.144	1.00 32.74
ATOM	4451		TIP	132		-13.172	18.733	1.00 58.65
MOTA	4452		TIP	133	45.301	11.497	21.408	1.00 35.00
ATOM	4453		TIP	134	57.705	-10.824	14.202	1.00 69.18
ATOM	4454		TIP	135	-3.108	15.385	16.685	1.00 38.07
ATOM	4455		TIP	136	85.884	11.182	9.044	1.00 32.04
ATOM	4456		TIP	137	12.840	-2.444	1.983	1.00 30.08
ATOM	4457		TIP	138	75.645	3.496	20.607	1.00 33.94
MOTA	4458		TIP	139	13.020	7.518	-2.510	1.00 40.68
ATOM	4459		TIP	140	11.245		0.729	1.00 26.02
ATOM	4460		TIP	141	59.563	10.829	14.466	1.00 71.34
ATOM	4461		TIP	142	13.671		3.489	1.00 39.47
ATOM	4462	OH2		143	-6.358	-3.421	16.520	1.00 37.08
ATOM	4463	OH2		144	25.629		3.534	1.00 50.51
ATOM	4464	OH2		145	-16.459	10.869	6.524	1.00 38.40
ATOM	4465	OH2		146	86.598	12.840	7.028	1.00 47.80
ATOM	4466	OH2	TIP	147	32.139	-4.674	1.757	1.00 32.43

ATOM	4467	OH2 TIP	148	44.890	7.505	11.806	1.00 32.46
MOTA	4468	OH2 TIP	149	80.781	12.432	16.562	
ATOM	4469	OH2 TIP	150	3.017	-7.101	-1.917	
MOTA	4470	OH2 TIP	151	31.784	-6.139	20.968	1.00 38.23
ATOM	4471	OH2 TIP	152	74.835	-2.597	12.290	1.00 48.89
ATOM	4472	OH2 TIP	153	7.509	6.768	-1.083	1.00 46.02
MOTA	4473	OH2 TIP	154	71.732	5.360	21.908	1.00 33.30
MOTA	4474	OH2 TIP	155	68.150	-5.075	8.794	1.00 39.31
MOTA	4475	OH2 TIP	156	0.148	-9.544	6.872	1.00 41.37
MOTA	4476	OH2 TIP	157	67.878	18.204	10.861	1.00 51.19
MOTA	4477	OH2 TIP	158	3.652	8.829	4.428	1.00 31.24
MOTA	:4478	OH2 TIP	159	52.100	11.362	18.433	1.00 40.73
MOTA	4479	OH2 TIP	161	-10.357	6.783	4.861	1.00 35.13
MOTA	4480	OH2 TIP	162	76.471	1.562	-0.853	1.00 59.17
ATOM	4481	OH2 TIP	163	10.073	-12.056	17.071	1.00 44.69
ATOM	4482	OH2 TIP	164	34.163	14.271	18.254	1.00 39.59
MOTA	4483	OH2 TIP	165	2.320	-7.990	16.820	1.00 38.19
MOTA	4484	OH2 TIP	166	29.696	1.908	6.098	1.00 38.02
ATOM	4485	OH2 TIP	167	32.626	-17.410	11.766	1.00 48.15
ATOM	4486	OH2 TIP	168	42.244	18.049	11.043	1.00 50.95
MOTA	4487	OH2 TIP	169	87.907	10.574	5.721	1.00 60.28
ATOM	4488	OH2 TIP	170	70.313	-3.998	25.141	1.30 72.64
MOTA	4489	OH2 TIP	171	77.603	5.679	23.952	1.00 43.23
ATOM	4490	OH2 TIP	172	-0.942	-8.153	4.508	1.00 55.10
ATOM	4491	OH2 TIP	173	34.297	15.574	1.690	1.00 34.19
ATOM	4492	OH2 TIP	174	-9.643	7.829	7.414	1.00 50.48
ATOM	4493	OH2 TIP	175	11.618	5.655	7.455	1.00 43.37
MOTA	4494	OH2 TIP	176	-8.705	13.841	13.642	1.00 72.49
ATOM	4495	OH2 TIP	177	32.009	3.416	18.257	1.00 44.16
ATOM	4496	OH2 TIP	178	-8.651	10.180	24.352	1.00 44.85
ATOM	4497	OH2 TIP	179	-1.153	-6.532	15.548	1.00 32.90
ATOM	4498	OH2 TIP	180	80.235	0.749	15.508	1.00 34.75
ATOM	4499	OH2 TIP	181	67.222	20.490	-1.574	1.00 40.76
MOTA	4500	OH2 TIP	182	-0.471	4.367	1.248	1.00 36.58
ATOM	4501	OH2 TIP	183	0.149	6.517	2.578	1.00 40.12
ATOM	4502	OH2 TIP	184	-1.186	8.867	1.311	1.00 44.77
ATOM	4503	OH2 TIP	185	-5.093	9.260	2.252	1.00 52.07
ATOM	4504	OH2 TIP	186	-7.235	10.227	3.913	1.00 58.53
ATOM	4505	OH2 TIP	187	2.724	7.169	0.879	1.00 47.77
MOTA	4506	OH2 TIP	188	5.527	11.031	8.519	1.00 34.40
ATOM	4507	OH2 TIP	189	63.927		22.689	1.00 40.75
ATOM	4508	OH2 TIP	190	79.264	1.066	18.321	1.00 41.34
ATOM ATOM	4509	OH2 TIP	191		-11.825	7.256	1.00 79.86
	4510	OH2 TIP	192	13.994	-0.972	-4.310	1.00 31.15
ATOM	4511	OH2 TIP	193	59.546	3.024	33.227	1.00 40.34
ATOM	4512	OH2 TIP	194	32.179	13.637	19.964	1.00 48.25
ATOM	4513	OH2 TIP	195	72.178	16.188	22.879	1.00 42.72
ATOM	4514	OH2 TIP	196	0.898	-8.663	14.348	1.00 41.76
ATOM	4515	OH2 TIP	197	-0.490	5.455	30.574	1.00 38.30
ATOM	4516	OH2 TIP	199	-1.277	-4.244	27.691	1.00 56.27
ATOM	4517	OH2 TIP	200	81.605	15.360	17.272	1.00 42.05
ATOM	4518	OH2 TIP	201	-17.534	4.081	23.779	1.00 59.65

ATON	4519	OH2 T	IP 202	27.748	10.634	14.595	1.00 49.97
ATOM	4 4520	OH2 T		34.891	4.468	27.604	1.00 60.26
ATOM	4 4521	OH2 T	IP 204	-3.460	-4.448	9.045	1.00 44.70
ATOM		OH2 T		42.705	7.590	22.526	1.00 35.77
ATOM		OH2 T		52.983	11.950	21.969	1.00 35.12
ATOM		OH2 T	IP 207	26.871	14.098	19.820	1.00 53.04
ATOM	4 4525	OH2 T	IP 208	-7.184	9.323	6.370	1.00 37.49
ATOM		OH2 T		86.676	5.553	15.911	1.00 72.92
ATOM		OH2 T		55.08 0	15.928	20.414	1.00 68.75
ATOM		OH2 T		51.512	19.264	22.672	1.00 54.72
ATOM		OH2 T		19.988	7.127	6.976	1.00 45.55
ATOM		OH2 T		28.905	2.021	-3.430	1.00 48.55
ATOM	1 4531	OH2 TI		26.446	2.593	-4.753	1.00 55.04
ATOM		OH2 T	P 215	36.539	2.911	18.446	1.00 38.50
ATOM		OH2 T	P 216	16.807	-20.725	14.119	1.00 56.03
ATOM		OH2 TI		28.203	-14.485	6.172	1.00 62.90
ATOM		OH2 TI		31.519	1.503	-2.010	1.00 56.19
ATOM		OH2 TI		10.014	-16.571	15.451	1.00 46.37
ATOM		OH2 TI			-11.922	5.526	1.00 56.89
ATOM		OH2 TI		-12.414	14.643	10.965	1.00 67.36
ATOM		OH2 TI		10.978	9.734	-1.436	1.00 38.81
ATOM		OH2 TI		11.293	12.362	-1.306	1.00 52.56
ATOM		OH2 TI		34.011	13.162	-1.255	1.00 52.58
ATOM		OH2 TI		31.195	17.923	8.021	1.00 75.88
ATOM		OH2 TI		36.957	11. 94 9	-1.947	3.00 50.98
ATOM		OH2 TI		35.179	3.114	10.888	1.00 58.55
ATOM		OH2 TI		64.027	13.281	26.577	1.00 51.98
ATOM		OH2 TI		36.514	6.155	15.292	1.00 45.57
ATOM		OH2 TI		90.627	4.339	6.386	1.00 56.65
ATOM		OH2 TI			-11.937	10.792	1.00 53.49
ATOM		OH2 TI			-10.212	16.610	1.00 79.85
ATOM		OH2 TI			-21.314	7.018	1.00 53.60
ATOM		OH2 TI		66.186	-1.068	30.882	1.00 56.92
ATOM ATOM		OH2 TI		75.153	18.983	20.700	1.00 34.22
ATOM		OH2 TI		-2.885	10.207	3.295	1.00 68.34
ATOM		OH2 TI		5.834	-3.507	25.370	1.00 34.75
ATOM				35.910	6.163	12.569	1.00 37.31
MOTA		OH2 TI		-5.494	16.637	14.033	1.00 65.17
ATOM		OH2 TI			-11.698	26.865	1.00 55.30
ATOM		OH2 TI		6.179	6.434	13.895	1.00 45.92
ATOM				-3.869		20.821	1.00 41.96
ATOM		OH2 TI		1.690 86.181	-3.598 11.454	-0.200	1.00 41.42
				90.191		23.000	1.00 56,22
		OH2 TI					
ATOM	4562	OH2 TI	P 245	10.501	7.621	5.627	1.00 77.40
ATOM ATOM	4562 4563	OH2 TI	P 245 P 246	10.501 5.007	7.621 8.485	5.627 2.181	1.00 77.40 1.00 89.31
ATOM ATOM ATOM	4562 4563 4564	OH2 TI OH2 TI OH2 TI	P 245 P 246 P 247	10.501 5.007 64.552	7.621 8.485 -8.093	5.627 2.181 20.595	1.00 77.40 1.00 89.31 1.00 45.86
MOTA MOTA MOTA	4562 4563 4564 4565	OH2 TI OH2 TI OH2 TI OH2 TI	P 245 P 246 P 247 P 248	10.501 5.007 64.552 11.243	7.621 8.485 -8.093 -17.828	5.627 2.181 20.595 13.332	1.00 77.40 1.00 89.31 1.00 45.86 1.00 65.30
MOTA MOTA MOTA MOTA MOTA	4562 4563 4564 4565 4566	OH2 TI OH2 TI OH2 TI OH2 TI	P 245 P 246 P 247 P 248 P 249	10.501 5.007 64.552 11.243 42.226	7.621 8.485 -8.093 -17.828 -6.785	5.627 2.181 20.595 13.332 14.857	1.00 77.40 1.00 89.31 1.00 45.86 1.00 65.30 1.00 81.78
ATOM ATOM ATOM ATOM ATOM	4562 4563 4564 4565 4566 4567	OH2 TI OH2 TI OH2 TI OH2 TI OH2 TI	P 245 P 246 P 247 P 248 P 249 P 250	10.501 5.007 64.552 11.243 42.226 2.875	7.621 8.485 -8.093 -17.828 -6.785 -4.176	5.627 2.181 20.595 13.332 14.857 22.032	1.00 77.40 1.00 89.31 1.00 45.86 1.00 65.30 1.00 81.78 1.00 53.45
ATOM ATOM ATOM ATOM ATOM ATOM	4562 4563 4564 4565 4566 4567 4568	OH2 TI	P 245 P 246 P 247 P 248 P 249 P 250 P 251	10.501 5.007 64.552 11.243 42.226 2.875 72.048	7.621 8.485 -8.093 -17.828 -6.785 -4.176 1.134	5.627 2.181 20.595 13.332 14.857 22.032 -2.037	1.00 77.40 1.00 89.31 1.00 45.86 1.00 65.30 1.00 81.78 1.00 53.45 1.00 38.85
ATOM ATOM ATOM ATOM ATOM	4562 4563 4564 4565 4566 4567 4568 4569	OH2 TI OH2 TI OH2 TI OH2 TI OH2 TI	P 245 P 246 P 247 P 248 P 249 P 250 P 251 P 252	10.501 5.007 64.552 11.243 42.226 2.875	7.621 8.485 -8.093 -17.828 -6.785 -4.176	5.627 2.181 20.595 13.332 14.857 22.032	1.00 77.40 1.00 89.31 1.00 45.86 1.00 65.30 1.00 81.78 1.00 53.45

MOTA	4571	OH2	TIP	255	43.306	20.459	30.366	1.00	47.59
MOTA	4572	OH2	TIP	256	67.064	16.514	15.765	1.00	57.51
MOTA	4573	OH2	TIP	257	87.612	21.648	5.147	1.00	70.52
MOTA	4574	OH2	TIP	258	21.095	9.853	-9.308	1.00	78.97
ATOM	4575	OH2	TIP	261	71.914	28.544	7.912	1.00	83.90
MOTA	4576	OH2	TIP	262	25.727	-8.133	27.190	1.00	54.87
MOTA	4577	OH2	TIP	263	-18.738	10.877	12.767	1.00	71.80
MOTA	4578	OH2	TIP	264	30.524	11.543	16.329	1.00	46.98
MOTA	4579	OH2	TIP	265	22.211	-16.242	-2.763	1.00	55.17
ATOM	4580	OH2	TIP	266	29.755	9.037	18.396	1.00	67.93
ATOM	4581	C1	MON	1000	67.458	4.500	11.935	1.00	0.00
ATOM	4582	C2	MON	1000	67.015	3.958	10.687	1.00	0.00
MOTA	4583	N3	MON	1000	67.367	2.732	10.160	1.00	0.00
ATOM	4584	C4	MON	1000	66.127	4.618	9.793	1.00	0.00
MOTA	4585	C5	MON	1000	65.620	5.919	10.125	1.00	0.00
MOTA	4586	C6	MON	1000	66.041	6.508	11.380	1.00	0.00
MOTA	4587	C7	MON	1000	66.948	5.809	12.276	1.00	0.00
ATOM	4588	C8	MON	1000	65.933	3.759	8.668	1.00	0.00
ATOM	4589	C10	MON	1000	66.745	2.518	8.922	1.00	0.00
MOTA	4590	C11	MON	1000	65.043	4.051	7.483	1.00	0.00
ATOM	4591	012	MON	1000	66.862	1.516	8.241	1.00	0.00
ATOM	4592		MON	1000	64.479	2.990	6.570	1.00	0.00
MOTA	4593		MON	1000	63.459	3.330	5.617	1.00	0.00
ATOM	4594		MON	1000	62.923	2.333	4.727	1.00	0.00
ATOM	4595		MON	1000	63.379	0.956	4.754	1.00	0.00
ATOM	4596		MON	1000	64.960	1.637	6.605	1.00	0.00
ATOM	4597		MON	1000	64.418	0.642	5.713	1.00	0.00
ATOM	4598		MON	1000	62.848	-0.025	3.880	1.00	0.00
ATOM	4599		MON	1000	63.429	-1.407	3.816	1.00	0.00
ATOM	4600		MON	1000	61.888	0.343	2.786	1.00	0.00
ATOM	4601	C22	MON	1000	61.085	-0.818	2.152	1.00	0.00
ATOM	4602		MON	1000	61.868	-2.035	1.930	1.00	0.00
ATOM	4603	C24		1000	62.562	-2.492	3.133	1.00	0.00
MOTA	4604	025		1000	61.481	-2.328	-0.389	1.00	0.00
ATOM	4605	C26		1000	62.001	-2.670	0.659	1.00	0.00
ATOM	4606	Cl	MON	1001	5.458	3.340	18.422	1.00	0.00
ATOM	4607	C2	MON	1001	6.049	3.475	19.718	1.00	0.00
ATOM	4608	N3	MON	1001	5.935	2.580	20.763	1.00	0.00
ATOM	4609	C4	MON	1001	6.857	4.573	20.124	1.00	0.00
ATOM	4610	C5	MON	1001	7.121	5.641	19.202	1.00	0.00
ATOM ATOM	4611 4612	C6	MON	1001	6.543	5.548	17.877	1.00	0.00
MOTA	4613	C7 C8	MON	1001	5.722	4.412	17.489	1.00	0.00
ATOM			MON	1001	7.250	4.340	21.477	1.00	0.00
ATOM	4614	C10		1001	6.647	3.023	21.886	1.00	0.00
	4615	C11		1001	8.138	5.242	22.302	1.00	0.00
ATOM ATOM	4616	012		1001	6.735	2.426	22.943	1.00	0.00
	4617	C13		1001	8.918	4.783	23.509	1.00	0.00
ATOM	4618	C14		1001	9.913	5.641	24.091	1.00	0.00
ATOM	4619	C15		1001	10.654	5.224	25.253	1.00	0.00
ATOM ATOM	4620	C16		1001	10.435	3.935	25.881	1.00	0.00
ATOM ATOM	4621	C17		1001	8.670	3.508	24.123	1.00	0.00
ATOM	4622	C18	MON	1001	9.416	3.095	25.285	1.00	0.00

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MOTA	4623	N19 MON	1001	11.168	3.525	27.023	1.00	0.00
MOTA	4624	C20 MON	1001	10.831	2.255	27.749	1.00	0.00
ATOM	4625	C21 MON	1001	12.107	4.463	27.725	1.00	0.00
MOTA	4626	C22 MON	1001	13.125	3.821	28.698	1.00	0.00
MOTA	4627	N23 MON	1001	12.570	2.742	29.518	1.00	0.00
ATOM	4628	C24 MON	1001	11.902	1.711	28.725	1.00	0.00
ATOM	4629	O25 MON	1001	13.118	3.569	31.669	1.00	0.00
MOTA	4630	C26 MON	1001	12.610	2.731	30.944	1.00	0.00

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CLAIMS

What is claimed is:

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1. A crystalline form of a polypeptide corresponding to the catalytic domain of a protein tyrosine kinase.

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2. The crystalline form of claim 1, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

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3. The crystalline form of claim 2, wherein said receptor protein tyrosine kinase is selected from the group consisting of PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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4. The crystalline form of claim 1, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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5. The crystalline form of claim 4, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

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6. The crystalline form of claim 1, comprising one or more heavy metal atoms.

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7. The crystalline form of claim 1, wherein said

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protein tyrosine kinase is FGFR.

8. The crystalline form of claim 7, wherein said FGFR is FGFR1.

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- 9. The crystalline form of claim 8, defined by atomic structural coordinates set forth in Table 1.
- 10. The crystalline form of claim 7, comprising at least one compound.
 - 11. The crystalline form of claim 10, wherein said compound is a nucleotide analog.

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12. The crystalline form of claim 11, wherein said nucleotide analog is AMP-PCP.

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13. The crystalline form of claim 12, defined by atomic structural coordinates set forth in Table 2.

14. The crystalline form of claim 10, wherein said compound is an indolinone compound.

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15. The crystalline form of claim 14, wherein said indolinone compound has a structure set forth in formula I or II:

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$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{4}$$

$$R_{6}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{4}$$

$$R_{6}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{3}$$

$$R_{6}$$

$$R_{5}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

- (a) A_1 , A_2 , A_3 , and A_4 are independently carbon or nitrogen;
 - (b) R₁ is hydrogen or alkyl;
- (c) R_2 is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
 - (d) R₃ is hydrogen;

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(e) R_4 , R_5 , R_6 , and R_7 are optionally present and are

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either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(0)R, SO_2NRR' , SO_3R , SR, NO_2 , NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, $(CH_2)_nCO_2R$, and CONRR' or (ii) any two adjacent R_4 , R_5 , R_6 , and R_7 taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

- (f) R₂', R₃', R₄', R₅', and R₆' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO₂NRR', SO₃R, SR, NO₂, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH₂)_nCO₂R, and CONRR';
- (g) n is 0, 1, 2, or 3;
 - (h) R is hydrogen, alkyl or aryl;
 - (i) R' is hydrogen, alkyl or aryl; and
- (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, 20 pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4oxadiazole, 1,2,3,4-oxatriazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 25 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO_2NRR' , SO_3R , SR, NO_2 , NRR', OH, CN, C(O)R, OC(O)R, 30 NHC(0)R, $(CH_2)_nCO_2R$ or CONRR'.

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- 16. The crystalline form of claim 15, wherein said indolinone compound is 3-[(3-(2-carboxyethyl)-4-methylpyrrol-5-yl)methylene]-2-indolinone.
- 5 17. The crystalline form of claim 15, wherein said indolinone compound is 3-[4-(4-formylpiperazine-1-yl)benzylidenyl]-2-indolinone.
- 18. The crystalline form of claim 16, defined by
 the atomic structural coordinates of Table 3.
 - 19. The crystalline form of claim 17, defined by the atomic structural coordinates of Table 4.
- 15 20. The crystalline form of claim 1, having monoclinic unit cells.

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- 21. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=208.3 Å, b=57.8 Å, c=65.5 Å and $\beta=107.2^{\circ}$.
- 22. The crystalline form of claim 20, wherein said monoclinic unit cells have dimensions of about a=211.6 Å, b=51.3 Å, c=66.1 Å and β =107.7°.
- 23. The crystalline form of claim 10, comprising one or more heavy metal atoms.
- 24. A polypeptide corresponding to the catalytic

 domain of a protein tyrosine kinase, containing at least
 about 20 amino acid residues upstream of the first

glycine in the conserved glycine-rich region of the catalytic domain, and at least about 17 amino acid residues downstream of the conserved arginine located at the C-terminal boundary of the catalytic domain.

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25. The polypeptide of claim 24, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

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26. The polypeptide of claim 24, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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27. The polypeptide of claim 25, wherein said receptor tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, KDR, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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28. The polypeptide of claim 26, wherein said non-receptor kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

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- 29. The polypeptide of claim 24 having the amino acid sequence shown in SEQ ID NO:4.
- 30. A method of using the polypeptide of claim 24 to form a crystal, comprising the steps of:
- (a) mixing a volume of polypeptide solution with a reservoir solution; and

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(b) incubating the mixture obtained in step(a) over the reservoir solution in a closed container,

under conditions suitable for crystallization.

- 31. A method of obtaining an FGF receptor tyrosine kinase domain polypeptide in crystalline form, comprising the steps of:
- (a) mixing a volume of polypeptide solution with an equal volume of reservoir solution, wherein said polypeptide solution comprises 1 mg/mL to 60 mg/mL FGF-type tyrosine kinase domain protein, 10 mM to 200 mM buffering agent, 0 mM to 20 mM dithiothreitol and has a pH of about 5.5 to about 7.5, and wherein said reservoir solution comprises 10% to 30% (w/v) polyethylene glycol, 0.1 M to 0.5 M ammonium sulfate, 0% to 20% (w/v) ethylene glycol or glycerol, 10 mM to 200 mM buffering agent and has a pH of about 5.5 to about 7.5; and
- (b) incubating the mixture obtained in step (a) over said reservoir solution in a closed container at a temperature between 0° and 25° °C until crystals form.

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32. The method of claim 31, wherein said polypeptide solution comprises about 10 mg/mL FGF receptor tyrosine kinase domain, about 10 mM sodium chloride, about 2 mM dithiothreitol, about 10 mM Tris-HCl and has a pH of about 8; the reservoir buffer comprises about 16% (w/v) polyethylene glycol (MW 10000), about 0.3 M ammonium sulfate, about 5% ethylene glycol or glycerol, about 100 mM bis-Tris and has a pH of about 6.5; and the temperature is about 4°C.

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33. The method of claim 31, wherein said

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polypeptide solution comprises a compound.

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- 34. A cDNA encoding an FGF receptor tyrosine kinase domain protein, wherein a coding strand of the cDNA has the nucleotide sequence of SEQ ID NO:5.
- 35. A method of determining three dimensional structures of protein tyrosine kinases with unknown structure comprising the step of applying structural atomic coordinates set forth in Table 1, Table 2, Table 3, or Table 4.
- 36. The method of claim 35, comprising the following steps:
- (a) aligning a first computer representation of an amino acid sequence of a protein tyrosine kinase of unknown structure with a second computer representation of a protein tyrosine kinase of known structure by matching homologous regions of amino acid sequences of said first computer representation and said second computer representation;
- (b) transferring computer representations of amino acid structures in said protein tyrosine kinase of known structure to computer representations of corresponding amino acid structures in said protein tyrosine kinase with unknown structure; and
- (c) determining a low energy conformation of the protein tyrosine kinase structure resulting from step (b).
 - 37. The method of claim 35, comprising the

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following steps:

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- (a) aligning the positions of atoms in the unit cell by matching electron diffraction data from two crystals; and
- (b) determining a low energy conformation of the resulting protein tyrosine kinase structure.
- 38. The method of claim 35, comprising the following steps:
- (a) determining the secondary structure of a protein tyrosine kinase structure using NMR data; and
- (b) simplifying the assignment of throughspace interactions of amino acids.
- 39. The method of any one of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a receptor protein tyrosine kinase.
- 40. The method of claim 39, wherein said receptor protein tyrosine kinase with or without known structure is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.
- 41. The method of anyone of claims 35, 36, 37, or 38, wherein said protein tyrosine kinase with or without known structure is a non-receptor protein tyrosine kinase.
- 30 42. The method of claim 41, wherein said protein tyrosine kinase with or without known structure is

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selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

- 43. A method of identifying a potential modulator of protein tyrosine kinase function by docking a computer representation of a structure of a compound with a computer representation of a structure of a cavity formed by the active-site of a protein tyrosine kinase, wherein said structure of said protein tyrosine kinase is defined by atomic structural coordinates set forth in Table 1, Table 2, Table 3, or Table 4.
- 44. The method of claim 43, comprising the following steps:
- (a) removing a computer representation of a compound complexed with a protein tyrosine kinase and docking a computer representation of a compound from a computer data base with a computer representation of the active-site of the protein tyrosine kinase;
- (b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and
- (c) identifying compounds that best fit said active-site as potential modulators of protein tyrosine kinase function.
- 45. The method of claim 43, comprising the following steps:
- (a) modifying a computer representation of compound complexed with a protein tyrosine kinase by the deletion of a chemical group or groups or by the

addition of a chemical group or groups;

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- (b) determining a conformation of the complex resulting from step (a) with a favorable geometric fit and favorable complementary interactions; and
- (c) identifying compounds that best fit the protein tyrosine kinase active-site as potential modulators of protein tyrosine kinase function.
- 46. The method of claim 43, wherein said method comprises the following steps:
- (a) removing a computer representation of a compound complexed with a protein tyrosine kinase; and
- (b) searching a data base for data base compounds similar to said compounds using a compound searching computer program or replacing portions of said compound with similar chemical structures from a data base using a compound construction computer program.
- 47. The method of any one of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.
- 48. The method of claim 47, wherein said receptor protein tyrosine kinase is selected from the group consisting of FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.
- 49. The method of anyone of claims 43, 44, 45, or 46, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

- 50. The method of claim 49, wherein said protein tyrosine kinase is selected from the group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.
- 5 51. a potential modulator of protein tyrosine kinase function identified by the method of any one of claims 43, 44, 45, or 46.
 - 52. The potential modulator of claim 51, wherein said modulator is selected from a computer data base.
 - 53. The potential modulator of claim 51, wherein said modulator is constructed from chemical groups selected from a computer data base.
 - 54. The potential modulator of protein tyrosine kinase function of claim 51, wherein said modulator is an indolinone compound of formula I or II:

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$$R_{5}$$

$$R_{6}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{4}$$

$$CR_{3}$$

$$R_{6}$$

$$R_{6}$$

$$R_{6}$$

$$R_{1}$$

$$R_{1}$$

$$R_{1}$$

$$R_{1}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{1}$$

$$R_{2}$$

$$R_{3}$$

$$R_{6}$$

$$R_{7}$$

$$R_{1}$$

$$R_{1}$$

$$R_{2}$$

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or a pharmaceutically acceptable salt, isomer, metabolite, ester, amide, or prodrug thereof, wherein

- (a) A_1 , A_2 , A_3 , and A_4 are independently carbon or nitrogen;
 - (b) R₁ is hydrogen or alkyl;
- (c) R_2 is oxygen in the case of an oxindolinone or sulfur in the case of a thiolindolinone;
 - (d) R₃ is hydrogen;

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(e) R₄, R₅, R₆, and R₇ are optionally present and are either (i) independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO₂NRR', SO₃R, SR, NO₂, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH₂)_nCO₂R, and CONRR' or (ii) any two adjacent R₄, R₅, R₆, and R₇ taken together form a fused ring with the aryl portion of the oxindole-based portion of the indolinone;

(f) R₂', R₃', R₄', R₅', and R₆' are each independently selected from the group consisting of hydrogen, alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO₂NRR', SO₃R,

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SR, NO₂, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH₂) $_n$ CO₂R, and CONRR';

- (g) n is 0, 1, 2, or 3;
- (h) R is hydrogen, alkyl or aryl;
- (i) R' is hydrogen, alkyl or aryl; and
- (j) A is a five membered heteroaryl ring selected from the group consisting of thiophene, pyrrole, pyrazole, imidazole, 1,2,3-triazole, 1,2,4-triazole, oxazole, isoxazole, thiazole, isothiazole, furan, 1,2,3-oxadiazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, 1,3,4-oxadiazole, 1,2,3,5-oxatriazole, 1,2,3-thiadiazole, 1,2,4-thiadiazole, 1,2,5-thiadiazole, 1,3,4-thiadiazole, 1,2,3,4-thiatriazole, 1,2,3,5-thiatriazole, and tetrazole, optionally substituted at one or more positions with alkyl, alkoxy, aryl, aryloxy, alkaryl, alkaryloxy, halogen, trihalomethyl, S(O)R, SO₂NRR', SO₃R, SR, NO₂, NRR', OH, CN, C(O)R, OC(O)R, NHC(O)R, (CH₂)_nCO₂R or CONRR'.
- 55. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, comprising the following steps:
 - (a) administering said potential modulator to cells;
 - (b) comparing the level of protein tyrosine kinase phosphorylation between cells not administered the potential modulator and cells administered said potential modulator; and
 - (c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on

the difference in the level of protein tyrosine kinase phosphorylation.

- 56. A method of identifying a potential modulator of protein tyrosine kinase function as a modulator of protein tyrosine kinase function, wherein said method comprises the following steps:
- (a) administering a preparation of said potential modulator to cells;

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- (b) comparing the rate of cell growth between cells not administered the modulator and cells administered the modulator; and
- (c) identifying said potential modulator as a modulator of protein tyrosine kinase function based on the difference in the rate of cell growth.
- 57. A method of treating a disease associated with a protein tyrosine kinase with inappropriate activity in a cellular organism, wherein said method comprises the steps of:
- (a) administering a modulator of protein tyrosine kinase function to the organism, wherein said modulator is in an acceptable pharmaceutical preparation; and
- (b) activating or inhibiting the protein tyrosine kinase function to treat the disease.
- 58. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a receptor protein tyrosine kinase.

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59. The method of claim 58, wherein said receptor protein tyrosine kinase is selected from the group containing FGF-R, PDGF-R, FLK, CCK4, MET, TRKA, AXL, TIE, EPH, RYK, DDR, ROS, RET, LTK, ROR1, and MUSK.

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60. The method of any one of claims 55, 56, or 57, wherein said protein tyrosine kinase is a non-receptor protein tyrosine kinase.

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61. The method of claim 60, wherein said non-receptor protein tyrosine kinase is selected from a group consisting of SRC, BRK, BTK, CSK, ABL, ZAP70, FES, FAK, JAK, and ACK.

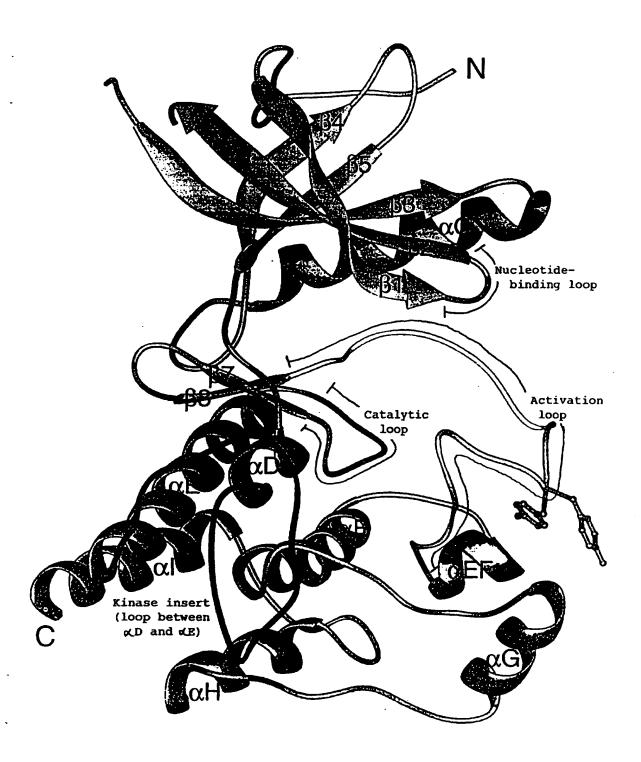
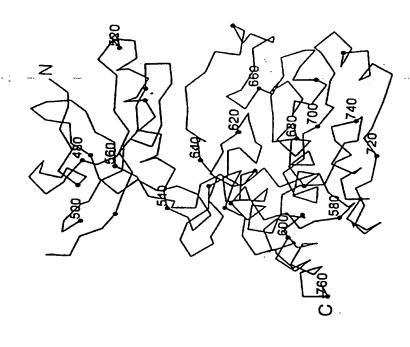
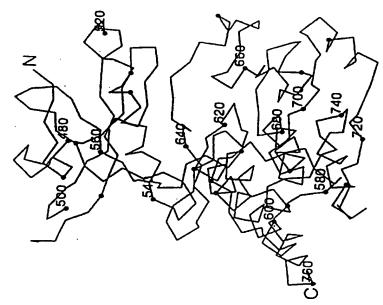


FIGURE 1







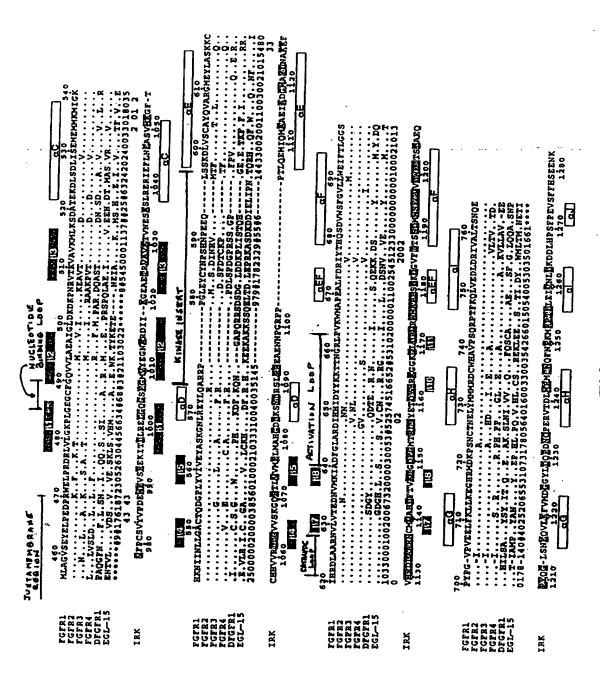
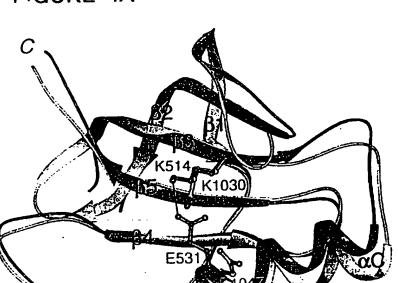
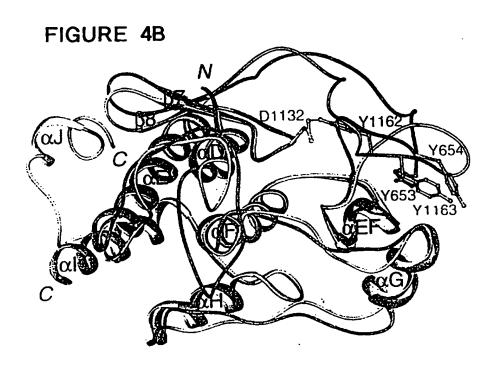


FIGURE 3

FIGURE 4A



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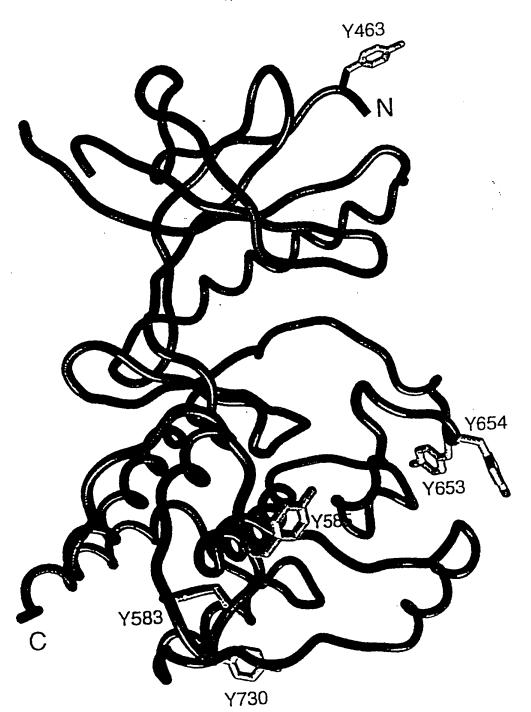


FIGURE 5

GLYCINE BICH

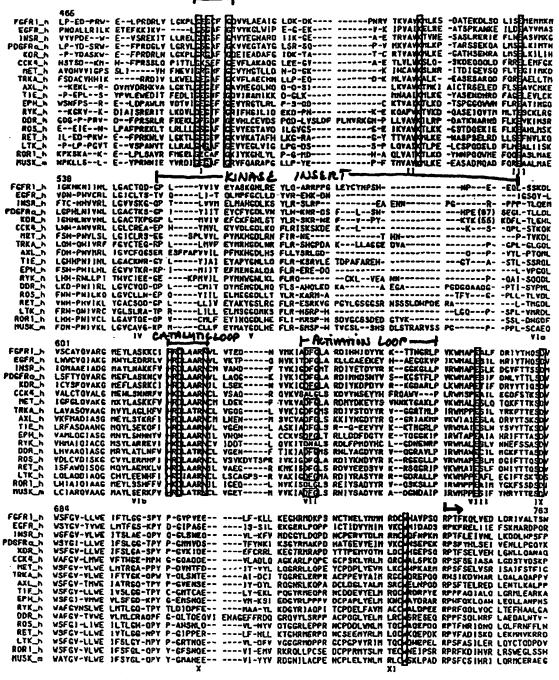


FIGURE 6A

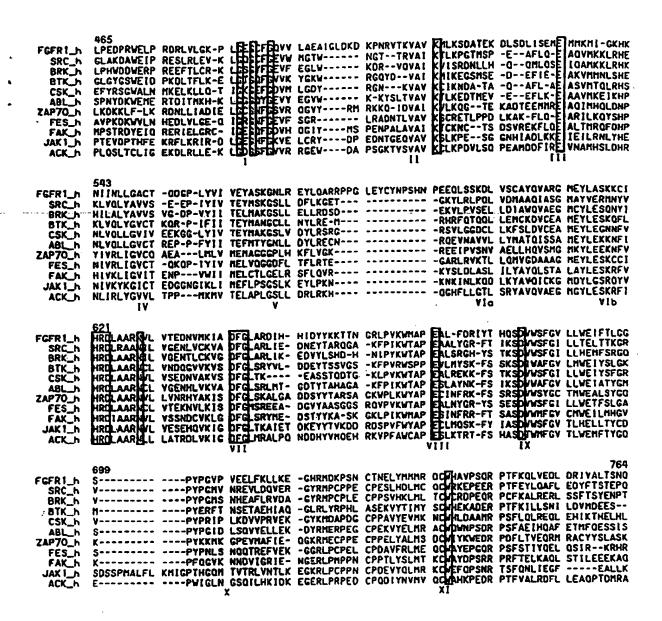


FIGURE 6B

	1	DRIYTHOSDV	HRIYTHOSHV	DGVFTTSSDM	DNLYTTLSDV	DRVYTIQSDV	EGDFSTKSDV	TOKFTTKSDV	YRKFTTESDV	DRVYTSKSDV	YSVYTTKSDV	HRIFTTASDV	NNEFSSASDV	MGKFTTASDV	DGIFTTQSDV	DHIYTTQSDV	EGIFTSKTDS	YGKFSSDSpI	YNRYTTESHV	XI
	ļ	VKWMAPERLF	IKWMALESIL	VRWMAPESLK	VKWMAPESIF	LKWMAPETIF	LRWMSPERIL	VKWMALESLO	IRWMPPESIL	VKWIAIESLA	VRWMAIESLN	IRWTAFERIA	VRWMALESLV	IRWMAWECIL	VRWMAPESLM	VKWMAIESLF	VKWMPPEAFL	IRWMPPERIM	IRWMPPESIF	VIII
LOOP		KTINGRLP	HAEGGKVP	KGGKGLLP	SKGSTFLP	RKGDARLP	FRQAWVP	VHNKTGAKLP	VGGRIMLP	QGRIAKMP	KKTMGRLP	ETQGGKIP	LGDNENRP	VQGRAVLP	KRGEGLLP	KRSQGRIP	RGDRALLP	VQSKSLLP	ADGNDAIP	
ACTIVATION LOOP		RDIHHIDYYK		RDIYETDYYR	RDIMHDSNYV	RDIYKDPDYV	KDVYNSEYYH	RDMYDKEYYS	RDIYSTDYYR	KKIYNGDYYR	RG-EEVYV	RLLDDFDGTY	RDLFPMDYHC	RNLYAGDYYR	RDIYKNDYYR	RDVYEEDSYV	RDIYRASYYR	REIYSADYYR	RNIYSADYYK	
_		VMKIADFGLA	HVKITDFGLA	TVKICDFGMT	IVKICEPECLA	WKICDEGLA	QVKVSALGLS	TVKVADFGLA	VVKICEPEMS	SVCVADFGLS	ASKIADFGLS	CCKVSDFGLT	QVKITDNALS	TIKIADFGMS	IVKICOFICLA	KMKISDFGLS	VAKICDEGMA	HVKISDLGLS	WKINDFOLS	VII
		VTEDN	VKTPQ	VAHDF	LAQGK	LSEKN	VSAQR	LDEKF	VGQGL	LNENM	VGENL	VNONL	IDDTL	VGENF	VSVKDYTSPR	VAEGR	LSCAGPSR	IGEQL	VGETM	
CATALYTIC , LOOP ,		ENGLAARIMI	HRDLAARWL	HRDLAARNCM	HRDLAARMVL	HRDLAARNIL	HKULAARACL	HRDLAARNCM	HRDLATRNCL	HRICLAARNCM	HRICLAARMVL	HRICLAARNIL	HKIDLAARNCV	HEDLATRACL	HRDLAARNCL	HRDLAARNIL	HRDIAARACL	HALLAARNIL	HRDLATRINCL]
		MEYLASKKCI	MNYLEDRRLV	MAYLNAKKFV	MEFLASKNCV	MEFLASRKCI	MEHLSNNRFV	MKYLASKKFV	MVYLAGLHFV	MEYLSTKRFI	MOYLSEKOFI	MNYLSNHNYV	MSYLARREVI	MRYLATLNFV	CVYLERMHFI	MOYLAEMKLV	CHYLEENHFI	MEYLSSHFFV	MAYLSERKFV	VID
·	601	VSCAYQVARG	LNWCVQIAKG	IOMAAEIADG	LSFTYOVARG	ICYSFOVAKG	VALCTOVALG		LAVASOVAAG	VKFMADIASG	LRFASDAANG	VAMLOGIASG	VHMAIOIACG	LHVAAQIASG	VDLCVDISKG	ISFAWOISOG	LOLAODIAOG	LHIAIOIAAG	LCIAROVAAG	•
		FGFR1_h	EGFR	INSR	PDGFRa h	KDR h	CCK4 h	MET	TRKA h	AXI. h	TIE	EPH h	RYKh	DDR_h	ROS	RET h	LTK	ROR1 h	MUSK m	

Fig. 6A-3

763 LDRIVALTSN	FSKMARDPOR	LKDDLHPSFP	VENLLPGQYK	LGNLLOANAO	LGDSTVDSKP	ISAIFSTFIG	LQALAQAPPV	LENTLKALPP	LGRMLEARKA	LEQLLANPHS	LTEFHAALGA	LAEDALNTV-	LOLFRNFFLN	LEKMMVKRRD	LOYCTODPDV	LRSWEGLSSH	LORMCERAEG	,
RDOWHAVESO RETEROLVED	RPKFRELIIE	RPTFLEIVNL	RPSFYHLSEI	RPTFSELVEH	RPSFSEIASA	RPSFSELVSR	RHSIKDVHAR	RPSFTELRED	RPPFAQIALQ		RPRFQQLVQC		RPTFHRIQNO	RPVFADISKD	RPSFASILER	RPRFKDIHVR	RPSFCSIHRI	
		RMCWDFNPKM	VKCWNSEPEK	LDCWHGEPSQ	ORCMALSPKD	LKCWHPKAEM	RGCWDREPOO	SRCWELNPOD	ROCWRDRPYE	KNOWAYDRAR	ACCWALDPEE	LRCWBRESEQ	TOCHAQEPDO	LOCWKOEPDK	TOCMDHEPEL	TECHNEIPSR	RLCWSKLPAD)
KEGHRMDKPS NCTNELYMM	ICTIDUYMIM	NCPERVTDLM	HATSEVYEIM	YTTPEMYQTM	GCPSKLYRLM	YCPDPLYEVM	ACPPEVYAIM	DCLDGLYALM	NCDDEVYELM	DCPAPLYELM	TCPDELFAVM	ACPOGLYELM	NCPDDLWNLM	NCSEEMYRLM	GCPGPVYRIM	DCPPRMYSLM	NCPLELYNLM	
		MDGGYLDQPD	KSGYRMAKPD	KEGTRMRAPD	AGKARLPQPE	LOGRRLLQPE	TQGRELERPR	RQGNRLKQPA	POGYRMEQPR	EDGYRLPPPV	KDGYRIAQPI	GRQVYLSRPP	OTGGRLEPPR	KTGHRMERPD	VGGGRMDPPR	RKRQLLPCSE	RDGNILACPE 1	
LF-KLL	IS-SIL	VL-KFV	TFYNKI	EFCRRL	VLADLO	IT-VYL	AI-DCI	IX-DYL	LY-EKL	VM-KSI	MAA-YL	ENAGEFFRDQ	VL-NYV	LF-NLL	VL-DFV	VI-EMV	VYY-IV	
P-GVPVEE	D-GIPASE	O-GISNEO	P-GMMVDS	P-GVKIDE	G-GQADDE	P-DVNTFD	Y-QLSNTE	P-GVENSE	C-GMTCAE	G-EMSNOE	TLDIDPFE	G-QLTDEQVI	P-AHSNLD	P-GIPPER	P-GRTNQE	Y-GFSNQE	Y-GMAHEE	×
IFTLGG-SPY	LMTFGS-KPY	ITSLAE-QPY	IFSLGG-TPY	IFSLGA-SPY	VFTHGE-MPH	LMTRGA-PPY	IFTYGK-QPW	IATRGQ-TPY	IVSLGG-TPY	VLSFGD-KPY	LMTLGQ-TPY	VLMLCRAQPF	ILTLGH-QPY	IVTLGG-NPY	IFSLGY-MPY	IFSFGL-QPY	IFSYGL-QPY	
684 WSFGV-LLWE	WSYGV-TVWE			WSFGV-LLWE	WAFGV-LMWE	WSFGV-VLWE	WSFGV-VLWE	WSFGV-TMWE	WSFGV-LLWE	WSFGI-VMWE	WAFGVNSLWE	WAFGV-TVWE	WSFGI-LIWE	WSFGV-LLWE	WSFGV-LLWE	WSFGV-VLWE	WAYGV-VLWE	
GFR1 h	EGFR_h	INSR_h	GFRa_h	KDR_h	CCK4_h				TIE_h	EPH_h	RYK_h	DDR_h	ROS_h	RET_h	LTK_h	ROR1_h	MUSK_m	

Fig. 6A-4

10/11

10/11	
465 LPEDPRWELP RDRLVLGK-P 1GBGCFGVV LAEAIGLDKD KPNRVTKVAV KMLKSDATEK DLSDLISEME MMXMI-GKHK GLAKDAWELP RESIRLEV-K 1GGGCFGEVW MGTW NGTTRVAI KTIKFGTMSP -EAFLQ-E AQVMKKLRHK GLAKDAWELP RESIRLEV-K 1GGGCFGEVW MGTW KDRVQVAI KVISRDNLLH -QQMLQSE IQAMKKLRHK GLGGGSWEID PKDLTFIK-E 1GTGGCFGVVK YGKW RGQYDVAI KMIKEGSMSE -DEFIE-E AKVMMNLSHE EFYRSGWALN MKELKLLQ-T IGKGEFGDVM LGDY RGNKVAV KTIKEDTMEV -BBFLK-E AAVWKEIKHP SPNYDKWEME RTDITMKH-K 1GGGCFGVV GGVY	543 NIINLLGACT -QDGP-LYVI VEYASKGNLR EYLQARRPPG LEYCYNPSHN PEEQLSSKDL VSCAYQVARG MEYLASKKCI KLVQLYAVVS -B-EP-IYIV TEYMSKGSLL BLLRDSDRKVLPVSEL LDIAWQVAEG MCYLESQNYI KLVQLYGVCT KQR-P-IFII TEYMANGCLL NYLRE-MRRVLGGDCL LKFSLDVCEA MEYLEGNNFV NLVQLLGVIV EEKGG-LYIV TEYMAKGSLV DYLRSRGRSVLGGDCL LKFSLDVCEA MEYLEGNNFV NLVQLLGVCT REP-P-FYII TEFMTYGNLL DYLRSRGRQEVNAVVL LYMATQISSA MEYLEEKNFI NLVQLLGVCT REP-P-FYII TEFMTYGNLL DYLRECNRQEVNAVVL LYMATQISSA MEYLEEKNFI NLVQLLGVCT REP-P-FYII TEFMTYGNLL DYLRECNRQEVNAVVL LYMATQISSA MEYLEEKNFV NLVQLLGVCT REP-P-TYII TEFMTYGNLL DYLRECNREEIPVSNV AELLHQVSMG MKYLEEKNFI NLVQLLGVCT -QKQP-IXIV MELVQGGDFL TFLRTE
FGFR1_h SRC_h BRK_h BIK_h CSK_h ABL_h ZAP70_h FES_h FAK_h	FGFR1_h SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h FAK_h JAK1_h

Fig. 6B-1

Fig. 6B-

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HRDLAARNUL VGENLVCKVA DFGLARLIE- DNEYTARQGA - KFPIKWTAP EALYGR-FT IKSDVWSFGI LLTELTTKGR HRDLAARNIL VGENLVCKVA DFGLARLIE- DNEYTARQGA - NIPYKWTAP EALSRGH-YS TKSDVWSFGI LLHEMFSRGQ HRDLAARNIL VGENLVCKVA DFGLARLIK- EDVYLSHD-H - KFPVKWAPP EVLMYSK-FS SKSDIWAFGV LWMEIYSLGK HRDLAARWUL VNDQGVVKVS DFGLSRYVL EASSTQDTG - KLPVKWTAP EALREKK-FS TKSDVWSFGI LLWEIATYGM HRDLAARWUL VSEDNVAKVS DFGLSRLMT- GDTYTAHAGA - KFPIKWTAP ESLAYNK-FS IKSDVWAFGV LIWELTSTGR HRDLAARWUL LVNRHYAKIS DFGLSKALGA DSYYTARSA GKWPLKWYAP EZIAYNK-FS SKSDVWSYGC TWWEALSYGQ HRDLAARWUL LVNRHYAKIS DFGLSKALGA DGSYYTARSA GKWPLKWAPP ERLNYGR-YS SESDVWNFGV CWWEILMHGV HRDLAARWUL VSSNDCVKLG DFGLSKYMB- DGVXAASGGS RQVPVKWTAP ESINFRK-FT SASDVWMFGV THEELLTYCD HRDLAARWUL VSSNDCVKLG DFGLSKYMB- DSTYYKA-SK GKLPIKWMAP ESINFRR-FT SASDVWMFGV TLHEELLTYCD HRDLAARWUL VSSNDCVKLG DFGLTKAIET DKEYYTVKDD RDSPVFWYAP ECLMQSK-FY HASDTWMFGV TLHEELLTYCD HRDLAARWUL VSSHDVWIG DFGLTKAIET DKEYYTVKDD RDSPVFWYAP ECLMQSK-FY HASDTWMFGV TLWEMFTYGC VIII	SPYPGVP VEELFKLLKE -GHRMDKPSN CTNELYMMMR DOWHAVPSOR PTFKQLVEDL DRIVALTSNG S
FGFR1_h SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h FAK_h AKK_h	FGFR1_h SRC_h BRK_h BTK_h CSK_h ABL_h ZAP70_h FES_h FAK_h